BIOINFORMATICS AND COMPUTATIONAL BIOLOGY PUBLICATIONS FROM INDIA

(2002 – mid-2007)

ALL INDIA INSTITUTE OF MEDICAL SCIENCES, NEW DELHI.

2007

Alam, M. T., Bora, H., Bharti, P. K., Saifi, M. A., Das, M. K., Dev, V., Kumar, A., Singh, N., Dash, A. P., Das, B., Wajihullah & Sharma, Y. D. (2007). Similar trends of pyrimethamine resistance-associated mutations in Plasmodium vivax and P. falciparum. Antimicrob. Agents Chemother. 51, 857-863.

Alam, M. T., Das, M. K., Dev, V., Ansari, M. A. & Sharma, Y. D. (2007). Identification of two cryptic species in the Anopheles (Cellia) annularis complex using ribosomal DNA PCR-RFLP. Parasitol. Res. 100, 943-948.

Alam, M. T., Das, M. K., Dev, V., Ansari, M. A. & Sharma, Y. D. (2007). PCR-RFLP method for the identification of four members of the Anopheles annularis group of mosquitoes (Diptera: Culicidae). Trans. R. Soc. Trop. Med. Hyg. 101, 239-244.

Sharma, D. & Tyagi, J. S. (2007). The value of comparative genomics in understanding mycobacterial virulence: Mycobacterium tuberculosis H37Ra genome sequencing – a worthwhile endeavour. J. Biosci. 32, 185-189.

2006

Ahmed, A., Lumb, V., Das, M. K., Dev, V., Wajihullah & Sharma, Y. D. (2006). Prevalence of mutations associated with higher levels of sulfadoxine-pyrimethamine resistance in Plasmodium falciparum isolates from Car Nicobar Island and Assam, India. Antimicrob. Agents Chemother. 50, 3934-3938.

Sarin, R. & Sharma, Y. D. (2006). Thioredoxin system in obligate anaerobe Desulfovibrio desulfuricans: Identification and characterization of a novel thioredoxin 2. Gene, 376, 107-115.

Mittra, P., Vinayak, S., Chandawat, H., Das, M. K., Singh, N., Biswas, S., Dev, V., Kumar, A., Ansari, M. A. & Sharma, Y. D. (2006). Progressive increase in point mutations associated with chloroquine resistance in Plasmodium falciparum isolates from India. J. Infect. Dis. 193, 1304-1312.

Ahmed, A., Das, M. K., Dev, V., Saifi, M. A., Wajihullah & Sharma, Y. D. (2006). Quadruple mutations in dihydrofolate reductase of Plasmodium falciparum isolates from Car Nicobar Island, India. Antimicrob. Agents Chemother. 50, 1546-1549.

Vinayak, S., Mittra, P. & Sharma, Y. D. (2006). Wide variation in microsatellite sequences within each Pfcrt mutant haplotype. Mol. Biochem. Parasitol. 147, 101-108.

Alam, M. T., Das, M. K., Ansari, M. A. & Sharma, Y. D. (2006). Molecular identification of Anopheles (Cellia) sundaicus from the Andaman and Nicobar islands of India. Acta Trop. 97, 10-18.

2004

Rawat, D. S., Sharma, I., Jalah, R., Lomash, S., Kothekar, V., Pasha, S. T. & Sharma, Y. D. (2004). Identification, expression, modeled structure and serological characterization of Plasmodium vivax histone 2B. Gene, 337, 25-35.

Ahmed, A., Bararia, D., Vinayak, S., Yameen, M., Biswas, S., Dev, V., Kumar, A., Ansari, M. A. & Sharma, Y. D. (2004). Plasmodium falciparum isolates in India exhibit a progressive increase in mutations associated with sulfadoxine-pyrimethamine resistance. Antimicrob. Agents Chemother. 48, 879-889.

Tyagi, J. S. & Sharma, D. (2004). Signal transduction systems of mycobacteria with special reference to M. tuberculosis. Curr. Sci. 86, 93-102.

Tyagi, J. S. & Saini, D. K. (2004). Did the loss of two-component systems initiate pseudogene accumulation in M. leprae? Microbiology, 150, 4-7.

* Sharma, D., Issac, B., Raghava, G. P. & Ramaswamy, R. (2004). Spectral repeat finder (SRF): identification of repetitive sequences using Fourier transformation. Bioinformatics, 20, 1405-1412.

2002

Tyagi, J. S. & Sharma, D. (2002). Genomic study of Mycobacterium tuberculosis and its clinical applications. Ind. J. Pediatr. 69, S29-S38.

Tyagi, J. S. & Sharma, D. (2002). M. smegmatis and tuberculosis. Trends Microbiol. 10, 68-69.

ANNA UNIVERSITY, CHENNAI.

2007

Richard, T., Krishnan, R., Sharmila, A. & Gautam, P. (2007). In silico identification of putative metal binding motifs. Bioinformatics, 23, 267-272.

2006

Yuan, X., Hu, Z. Z., Wu, H. T., Torii, M., Narayanaswamy, M., Ravikumar, K. E., Vijay-Shanker, K. & Wu, C. H. (2006). An online literature mining tool for protein phosphorylation. Bioinformatics, 22, 1668-1669.

Madan, B. M., Leena, P. M., Tamil, S. A., Martin, M., Julian, G, Aravind, L. & Sankaran, K. (2006). A Database of Bacterial Lipoproteins (DOLOP) with Functional Assignments to Predicted Lipoproteins. J. Bacteriol. 188, 2761-2773.

Sharmila, A., Ramesh, A. & Gautam, P. (2006). Understanding mutations and protein stability through tripeptides. FEBS Lett. 580, 2071-2082.

Aswin, S. N. S., Krishnan, R., Karthikeyan, S. & Gautam, P. (2006). Role of Hydrophobic Interactions and Salt-Bridges in beta Hairpin Folding. J. Mol. Mod. 12, 197-205.

2005

Hu, Z. Z., Narayanaswamy, M., Ravikumar, K. E., Vijay-Shanker, K. & Wu, C. H. (2005). Literature mining and database annotation of protein phosphorylation using a rule-based system. Bioinformatics, 21, 2759-2765.

Sharmila, A., Mridula, P. & Pennathur, G. (2005). Potential Drug Targets in Mycobacterium tuberculosis through Metabolic Pathway Analysis. Comput. Biol. Chem. 29, 368-379 .

Subbulakshmi, L. C., Aswin, S. N. S., Krishnan, R., Sharmila, A. & Gautam, P. (2005). Evidence of a Double-Lid Movement in Pseudomonas aeruginosa Lipase: Insights from Molecular Dynamics Simulations. PLoS Comput. Biol. 1, e28.

Karthikeyan, S., Aswin, S. N. S., Krishnakumar, S., Geetha, M. & Gautam, P. (2005). Promoter Addresses: Revelations from Oligonucleotide Profiling Applied to the Escherichia coli genome. Theor. Biol. Med. Model. 2, 20.

2004

Anuradha, V., Sharmila, A. & Gautam, P. (2004). Functionally Specified Protein Signatures for Individual Blue Copper Proteins and for a Combination of Blue and Green and Blue and Purple Copper Proteins. BMC Bioinformatics, 5, 127.

2003

Jayasunder, J. J., Baddireddy, S. L., Venkateshamoorthy, R., Madhuranthagam, J. A., Pandjassarame, K. & Gautam, P. (2003). Insights from Molecular Dynamics Simulation into pH Dependent Enantio-Selective Hydrolysis of Esters by Candida rugosa Lipase. Protein Eng. 16, 1017-1024.

2002

Babu, M. M., Kamalakkannan, S., Subrahmanyam, Y. & Krishnan, S. K. (2002). Shigella apyrase a novel variant of bacterial acid phosphatases. FEBS Lett. 512, 8-12.

Babu, M. M. & Sankaran, K. (2002). DOLOP—database of bacterial lipoproteins. Bioinformatics, 18, 641-643.

Sharmila, A., Pennathur, G. & Ramesh, A. (2002). Tripeptide Analysis of Protein Structures. BMC Struct. Biol. 2, 9.

BANASTHALI VIDYAPITH, BANASTHALI.

2007

Shanker, A., Bhargava, A., Bajpai, R., Singh, S., Srivastava, S. & Sharma, V. (2007). Bioinformatically mined simple sequence repeats in unigene of Citrus sinensis. Sci. Horti. (In press).

Shanker, A., Kumar, A., Sangwan, C., Chowdhary, N., Gupta, S., Sonica & Sharma V. (2007). Orthologous and Essential Genes Identification in Cryptococcus neoformans and Neurospora crassa in Joint Indo Korean Symposium On Biochemical Engineering & Biotechnology, 22nd – 24th February, New Delhi, India.

2006

Shanker, A., Singh, A. & Sharma, V. (2006). In silico mining in expressed sequences of Neurospora crassa for identification and abundance of microsatellites. Microbiol. Res. (In press).

Shanker, A., Tripathi, D., Khandelwal, G., Sharma, G., Agrawal, S., Singh, A. & Sharma, V. (2006). Data mining and database development for simple sequence repeats of Takifugu rubripes (Japanese Pufferfish). Biochem. Cell. Arch. 6, 1-12.

BHARATHIDASAN UNIVERSITY, TRICHY.

2006

Premanandh, J., Priya, B., Teneva, I., Dzhambazov, B., Prabaharan D. & Uma L. (2006). Molecular Characterization of Marine Cyanobacteria from the Indian Subcontinent Deduced from Sequence Analysis of the Phycocyanin Operon (cpcB-IGS-cpcA) and 16S-23S ITS Region. J. Microbiol. 44, 607-616.

BOSE INSTITUTE, KOLKATA

2007

Mukhopadhyay, P., Basak, S. & Ghosh, T. C. (2007). Synonymous codon usage in different protein secondary structural classes of human genes: Implication for increased non-randomness of GC3 rich genes towards protein stability. J. Biosci. (In press).

Kahali, B., Basak, S. & Ghosh, T. C. (2007). Reinvestigating the codon and amino acid usage of S. cerevisiae genome: A new insight from protein secondary structure analysis. Biochem. Biophys. Res. Commun. 354, 693-699.

Sau, K., Gupta, S.K., Sau, S., Mandal, S.C. & Ghosh, T.C. (2007). Studies on synonymous codon and amino acid usage biases in the broad-host range bacteriophage KVP40. J. Microbiol. 45, 58-63.

Guharoy, M. & Chakrabarti, P. (2007). Secondary structure based analysis and classification of biological interfaces: identification of binding motifs in protein-protein interactions. Bioinformatics (In press).

Chakrabarti, P. & Bhattacharyya, R. (2007). Geometry of nonbonded interactions involving planar groups in proteins. Prog. Biophys. Mol. Biol. (In press).

* Vidyasagar, M. et al. (The NMITLI-BioSuite Team). (2007). BioSuite: a comprehensive bioinformatics software package (A unique industry-academia collaboration). Curr. Sci. 92, 29-38.

Janin, J., Rodier, F., Chakrabarti, P. & Bahadur, R. (2007). Macromolecular recognition in the Protein Data Bank. Acta Cryst. D63, 1-8.

Pal, A., Chakrabarti, P., Bahadur, R., Rodier, F. & Janin, J. (2007). Peptide segments in protein-protein interfaces. J. Biosci. 32, 101-111.

Saha, R. P., Bhattacharyya, R. & Chakrabarti, P. (2007). Interaction geometry involving planar groups in protein-protein interfaces. Proteins, 67, 84-97.

Roy, D. & Sengupta, S. (2007). Structural Features of a cold-adapted Alaskan bacterial Lipase. J. Biomol. Struct. Dyn. 24, 463-470.

Karmakar, R. & Bose, I. (2007). Positive feedback, stochasticity and genetic competence. Phys. Biol. 4, 29-37.

2006

Bagchi, A & Ghosh, T.C. (2006). Structural and functional characterization of SoxW – a thioredoxin involved in the transport of reductants during sulfur oxidation by the global sulfur oxidation reaction cycle. Res. J. Microbiol. 1, 392-400.

Basak, S. & Ghosh, T.C. (2006). Temperature adaptation of synonymous codon usage in different functional categories of genes: a comparative study between Methanococcus jannaschii and Methanococcus maripaludis homologous genes. FEBS Lett. 580, 3895-3899.

* Bagchi, A. & Ghosh, T.C. (2006). Structural study of two proteins SigE and ORF1 to predict their roles in the biochemical oxidation of sulfur anions via the global sulfur oxidation operon (sox). Comput. Biol. Chem. 30, 227-232.

Joy, F., Basak, S., Gupta, S. K., Das, P. J., Ghosh, S. K. & Ghosh. T.C. (2006). Compositional correlations in canine genome reflects similarity with human genes. Res. J. Microbiol. 1, 172-182.

Ghosh, T. C. (2006). Structural identification of the interactions of SoxA and SoxX during the oxidation of sulfur anions via the novel global sulfur oxidizing (Sox) operon. J. Biochem. Mol. Biol. 39, 240-246.

Sau, K., Gupta, S. K., Sau, S., Mandal, S. C., & Ghosh, T. C. (2006). Factors influencing synonymous codon and amino acid usage biases in Mimivirus. BioSystems, 85, 107-113.

Banerjee, T. & Ghosh, T.C. (2006). Gene expression level shapes the amino acid usages in Prochlorococcus marinus MED4. J. Biomol. Struct. Dyn. 23, 547-554.

Saha, R.P. & Chakrabarti, P. (2006). Molecular modeling and characterization of Vibrio cholerae transcription regulator HlyU. BMC Struct. Biol. 6, 24.

Saha, R.P., Bahadur, R., Pal, A., Mandal, S & Chakrabarti, P. (2006). ProFace: a server for the analysis of the physicochemical features of protein-protein interfaces. BMC Struct. Biol. 6, 11.

Raichaudhuri, A., Bhattacharyya, R., Chaudhuri, S., Chakrabarti, P. &. DasGupta, M. (2006). Domain analysis of a groundnut calcium-dependent protein kinase: nuclear localization sequence in the junction domain is coupled with nonconsensus calcium binding domains. J. Biol. Chem. 281, 10399-10409.

Saha, R.P. & Chakrabarti, P. (2006). Parity in the number of atoms in residue composition in proteins and contact preferences. Curr. Sci. 90, 558-561.

Bhattacharyya, R., Bhattacharya, S. & Choudhuri, S. (2006). Conservation and documentation of the medicinal plant resources of India. Biodiv. Conserv. 15, 2705-2717.

Chattopadhyay, S., Sinha, N.K., Banerjee, S., Roy, D., Chattopadhyay, D. & Roy, S. (2006). Small cationic protein from a marine turtle has beta-defensin-like fold and antibacterial and antiviral activity. Proteins, 64, 524-531.

Ghosh Dastidar, K., Maitra, S., Goswami, L., Roy, D., Das, K.P. & Majumder, A.L. (2006). An insight into the molecular basis of salt tolerance of L-myo-inositol 1-P synthase (PcINO1) from Porteresia coarctata (Roxb) Tateoka, a halophytic wild rice. Plant Physiol. 140, 1279-1296.

Ghosh, B. & Bose, I. (2006). Gene copy number and cell cycle arrest. Phys. Biol. 3, 29-36.

Karmakar, R. & Bose, I. (2006). Stochastic model of transcription factor-regulated gene expression. Phys. Biol. 3, 200-208.

2005

Bagchi, A. & Ghosh, T.C. (2005). Structural insight into the interactions of SoxV, SoxW and SoxS in the process of transport of reductants during sulfur oxidation by the novel global sulfur oxidation reaction cycle. Biophys. Chem. 119, 7-13.

Bagchi, A. & Ghosh T.C. (2005). Structural identification of a novel thioredoxin SoxS: prediction of the function in the process of transport of reductants during sulfur oxidation by the novel global sulfur oxidation reaction cycle. J. Mol. Struct. Theochem. 758, 113-118.

Banerjee, T., Gupta, S.K. & Ghosh, T.C. (2005). Compositional transitions between Oryza sativa and Arabidopsis thaliana genes are linked to the functional change of encoded proteins. Plant Sci. 170, 267-273.

* Bagchi, A. & Ghosh, T.C. (2005). A structural study towards the understanding of the interactions of SoxY, SoxZ and SoxB leading to the oxidation of sulfur anions via the novel global sulfur oxidizing (sox) operon Biochem. Biophys. Res. Commun. 335, 609-615.

Sahu, K., Sau, S., Mandal, S. C. & Ghosh, T.C. (2005). Factors influencing the synonymous codon and amino acid usage bias in an AT-rich P. aeruginosa phage PhiKZ. Acta Biochim. Biophys. Sin. 37, 625-633.

Gupta, S.K., Banerjee, T., Basak, S., Sahu, K., Sau, S., & Ghosh, T.C. (2005). Studies on codon usage in Thermoplasma acidophilum and its possible implications on the occurrences of lateral gene transfer. J. Basic Microbiol. 45, 344-354.

Sahu, K., Gupta, S. K., Sau, S. & Ghosh, T. C. (2005). Synonymous codon usage bias in 16 Staphylococcus aureus phages: Implication in phage therapy. Virus Res. 113, 123-131.

Sahu, K., Gupta, S.K., Sau, S. & Ghosh, T. C. (2005). Comparative analysis of the base composition and codon usages in fourteen mycobacteriophage genomes. J. Biomol. Struct. Dyn. 23, 63-72.

Banerjee, T., Gupta, S.K. & Ghosh, T.C. (2005). Role of mutational bias and natural selection on genome-wide nucleotide bias in prokaryotic organisms. BioSystems, 81, 11-18.

Basak, S. & Ghosh, T.C. (2005). On the origin of genomic adaptation at high temperature for prokaryotic organisms. Biochem. Biophys. Res. Commun. 330, 629-632.

Banerjee, T., Gupta, S.K. & Ghosh, T.C. (2005). Towards a resolution on the inherent methodological weakness of the "effective number of codons used by a gene". Biochem. Biophys. Res. Commun. 330, 1015-1018.

D'Onofrio, G. & Ghosh, T.C. (2005). The compositional transition of vertebrate genomes: an analysis of the secondary structure of the proteins encoded by human genes. Gene, 345, 27-33.

Basak, S., Mandal, S. & Ghosh, T. C. (2005). Correlations between genomic GC levels and optimal growth temperatures: some comments. Biochem. Biophys. Res. Commun. 327, 969-970.

Guharoy, M. & Chakrabarti, P. (2005). Conservation and relative importance of residues across protein-protein interfaces. Proc. Natl. Acad. Sci. USA, 102, 15447-15452.

Saha, R.P., Bahadur, R.P. & Chakrabarti, P. (2005). Interresidue contacts in proteins and protein-protein interfaces and their use in characterizing the homodimeric interface. J. Proteome Res. 4, 1600-1609

Rodier, F., Bahadur, R.P., Chakrabarti, P. &. Janin, J. (2005). Hydration of protein-protein interfaces. Proteins, 60, 36-45.

Pal, L., Dasgupta, B. & Chakrabarti, P. (2005). 3_{10}-helix adjoining α-helix and β-strand: sequence, structural features and their conservation. Biopolymers, 78, 147-162.

Gupta, S., Banerjee, M., Poddar, A., Banerjee, A., Basu, G., Roy, D. & Bhattacharya, B. (2005). The biphasic kinetics of Colchicine-Tubulin interaction: Role of amino acids surrounding the A-ring of bound colchicine molecule. Biochemistry, 44, 10181-10188.

* Bagchi, A., Roy, D. & Roy, P. (2005). Homology modeling of a transcriptional regulator SoxR of the lithotrophic sulfur oxidation (Sox) operon in α-Proteobacteria. J. Biomol. Struct. Dyn. 22, 571-577.

Ghosh, B., Karmakar, R. & Bose, I. (2005). Noise Characteristics of Feed Forward Loops. Phys. Biol. 2, 36-45.

2004

Basak, S., Banerjee, T., Gupta, S.K. & Ghosh, T.C. (2004). Investigation on the Causes of Codon and Amino Acid Usages Variation between Thermophilic Aquifex aeolicus and Mesophilic Bacillus subtilis. J. Biomol. Struct. Dyn. 22, 205-214.

Banerjee, T., Basak, S., Gupta, S.K. & Ghosh, T.C. (2004). Evolutionary forces in shaping the codon and amino acid usages in Blochmannia floridanus. J. Biomol. Struct. Dyn. 22, 13-24.

Sau, K., Gupta, S. K., Ghosh, T. C. & Sau, S. (2004). Synonymous codon usage analysis of mycobacteriophage Bxz1 and its plating bacteria M. smegmatis: identification of highly and lowly expressed genes of Bxz1 and the possible function of its tRNA species. J. Biochem. Mol. Biol. 37, 487-492.

Subramaniyam, V., Gupta, S. K. & Ghosh, T. C. (2004). Shannon's uncertainty principle and gene expression levels. Curr. Sci. 86, 1142-1147.

Gupta, S. K., Bhattacharyya, T. K. & Ghosh, T. C. (2004). Synonymous codon usage in Lactococcus lactis: Mutational Bias Versus Translational Selection. J. Biomol. Struct. Dyn. 21, 527-535.

* Bhattacharyya, R., Pal, D. & Chakrabarti, P. (2004). Disulfide bonds, their stereospecific environment and conservation in protein structures. Protein Eng. Design Selection, 17, 795-808.

Bahadur, R.P., Chakrabarti, P., Rodier, F. & Janin, J. (2004). A dissection of specific and non-specific protein-protein interfaces. J. Mol. Biol. 336, 943-955.

Dasgupta, B., Pal, L., Basu, G. & Chakrabarti, P. (2004). Expanded turn conformations: characterization and sequence-structure correspondence in α-turns with implications in helix folding. Proteins, 55, 305-315.

Roy, D. & Lohia, A. (2004). Sequence divergence of Entamoeba histolytica tubulin is responsible for its altered tertiary structure. Biochem. Biophys. Res. Commun. 319, 1010-1016.

Banerjee, S., Hess, D., Majumder, P., Roy, D. & Das, S. (2004). The interactions of allium sativum leaf agglutinin with a chaperonin group of unique receptor protein Isolated from a bacterial endosymbiont of the mustard aphid. J. Biol. Chem. 279, 23782-23789.

Karmakar, R. & Bose, I. (2004). Graded and binary responses in stochastic gene expression, Phys. Biol. 1, 197-204.

2003

Gupta, S.K. & Ghosh, T.C. (2003). Reinvestigation on the causes of genomic GC variation between the orthologous genes of Mycobacterium tuberculosis and Mycobacterium leprae. Biochem. Biophys. Res. Commun. 303, 65-68.

Bhattacharyya, R. & Chakrabarti, P. (2003). Stereospecific interactions of proline residues in protein structures and complexes. J. Mol. Biol. 331, 925-940.

Bahadur, R.P., Chakrabarti, P., Rodier, F. & Janin, J. (2003). Dissecting subunit interfaces in homodimeric proteins. Proteins, 53, 708-719 .

Bhattacharyya, R., Saha, R., Samanta, U. & Chakrabarti, P. (2003). Geometry of interaction of histidine ring with other planar and basic residues. J. Proteome Res. 2, 255-263 .

Pal, L., Chakrabarti, P. & Basu, G. (2003). Sequence and structure patterns in proteins from an analysis of the shortest helices: implications for helix nucleation. J. Mol. Biol. 326, 273-291.

Roy, D., Ghosh, D. & Gupta-Bhattacharya, S. (2003). Homology modeling of allergenic cyclophilins: IgE-binding site and structural basis of cross-reactivity. Biochem. Biophys. Res. Commun. 307, 422-429.

Bose, I. & Karmakar, R. (2003). Simple models of plant learning and memory. Phys. Scr. T106, 9-12.

2002

D'Onofrio, G., Ghosh, T.C. & Bernardi, G. (2002). The base composition of the human genes is correlated with the secondary structures of the encoded proteins. Gene, 300, 179-187.

Gupta, S.K., Bhattacharyya, T.K. & Ghosh, T.C. (2002). Compositional correlation and codon usage studies in Buchnera aphidicola. Ind. J. Biochem. Biophys. 39, 35-48.

* Bhattacharyya, R., Pal, D. & Chakrabarti, P. (2002). Secondary structures at polypeptide chain-termini and their features. Acta Cryst. D56, 1793-1802.

Samanta, U., Bahadur, R.P. & Chakrabarti, P. (2002). Quantifying the accessible surface area of protein residues in their local environment. Protein Eng. 15, 659-667.

Pal, L., Basu, G & Chakrabarti, P. (2002). Variants of 3_{10}-helices in proteins. Proteins, 48, 571-579.

Chakrabarti, P. & Janin, J. (2002). Dissecting protein-protein recognition sites. Proteins, 47, 334-343.

* Pal. D & Chakrabarti, P. (2002). On residues in the disallowed region of the Ramachandran map. Biopolymers, 63, 195-206.

Bhattacharyya, R., Samanta, U. & Chakrabarti, P. (2002). Aromatic–aromatic interactions in and around α-helices. Protein Eng. 15, 91-100.

CENTRAL DRUG RESEARCH INSTITUTE, LUCKNOW.

2007

Mishra, J.K., Garg, P., Doohare, P., Kumar, A., Siddiqi, M.I. Ray, M. & Panda,G. (2007).Amino acid based enanotiomerically pure 3-substituted benzondiazepine-ones: a new class of anti-ischemic agents. Bioorg. Med. Chem. Lett. 17, 1326-1331.

Kumar, A., Saeed, U. & Siddiqi, M.I. (2007). Molecular Docking and 3-D QSAR Studies of Human Mitotic Kinesin Eg5 Inhibitors. Med.Chem.Res. 15,243.

Naim,M., Bhat,S., Rankini,K.N., Dennis, S., Chowdhury, S.F., Siddiqi, M.I., Drabik, P., Sulea T., Bayly,C., Jakalian, A. & Purisima, E.O. (2007). Solvated interaction energy (SIE) for scoring protein-ligand binding affinities. 1. Exploring the parameter space. J. Chem. Info. Model. 47, 122-133.

Rawal, R.K., Kumar, A., Siddiqi, M.I. & Katti, S.B. (2007). Molecular Docking Studies on 4-Thiazolidinones as HIV-1 RT Inhibitors, J. Mol. Model, 13, 155-161.

Shagufta, Ashutosh, K., Gautam, P. & Siddiqi, M.I. (2007). CoMFA and CoMSIA based 3D-QSAR Analysis of Diaryloxy methano phenanthrene Analogues as Anti-tuberculosis Agents. J. Mol. Model. 13, 99-109.

Srivastava, S.K., Dube, D., Vandna, K., jha, A.K., Hajela, K. & Ravishankar, R. (2007). NAD+ -dependent DNA ligas(Rv3014c) from Mycobacterium tuberculosis : Novel structure-function relationship and identification of a specific inhibitor. Proteins: Struct. Funct. Bioinfo. 69, 97-111.

Divya, D., Sarvind, M. T. & Ravishankar, R. (2007). Identification of inhibitors of M.tuberculosis Lysine 3-aminotransferase by Virtual screening. Med. Chem. Res. 15,181.

Divya, D., Sandeep, K., Srivastava, Vanda, K., Rama, P.T. & Ravishankar R. (2007). Novel specific inhibitors of NAD+ -dependent DNA ligase (Rv3014c) identified from virtual screening. Med. Chem. Res. 15, 93.

Raghu, R., EVS Kumar, A., Biswas, S., Kumar, A., Chaubey, S., Siddiqi, M.I. & Habib, S. (2007). Nuclear gyrB encodes a functional subunit of the Plasmodium falciparum gyrase that is ionvolved in apicoplast DNA replication. Mol. Biochem. Parasit. 154, 30-39.

Agrawal, H., Kumar, A., Bal, N.C., Siddiqi M.I., and Arora, A. (2007). Ligand based Virtual Screeening and Biological Evalution of Inhibitors of Chorismate Mutase (Rv1885c) from Mycobacterium tuberculosis H37Rv. Bioorg. Med. Chem. Lett. 17, 3053-3058.

2006

Lakshmi, M., Dixit, A. & Saxena, A. K. (2006). QSAR studies on cis-hexa and tetrahydrophthalaziones: A new class of PDE-4 inhibitors. Indian J. Chem. 45A, 34-45.

Saxena, A. K. & Schaper, K. J. (2006). QSAR analysis of the time- and dose-dependent anti-inflammatory in vivo activity of substituted imidazo[1,2-a] pyridines using artificial neural networks. QSAR & Combinatorial Science. 25, 590-597.

Saxena, A. K. & Prathipati, P. (2006). Collection and preparation of molecular databases for virtual screening. SAR & QSAR Environ. Res. 17, 371-392.

2005

Rao, j., Chakraborty, R., Roy, R., Mishra, A. & Saxena, A. K. (2005). A Convenient stereospecific synthesis of substituted 1,2,3,4,6,6a,7,11b,12,12a-decahydropyrazino-[1',2':1,6]pyrido[3,4-b]indoles. Arkivoc, 2, 20-28.

Srivastava, S.K., Dube, D., Tewari, N., Dwivedi, N., Tripath, R.P. & Ravishankar, R. (2005). Mycobacterium tuberculosis NAD^+ -dependent DNA ligase is selectively inhibited by glycosylamines compared with human DNA ligase 1. Nucl. Acids Res. 33, 7090-7101.

Srivastava, S. K., Tripati, R. P. & Ravishankar, R. (2005). NAD^+-dependent DNA ligase(rv3014c) from M.tuberculosis:Crystal structure of the adenylation domain and identification of novel inhibitors, J. Biol. Chem. 280, 30273-30281.

2004

Dixit, A., Kashaw, S.K., Gaur, S. & Saxena, A.K. (2004). Development of CoMFA, advance CoMFA and CoMSIA models in pyrroloquinazolines as thrombin receptor antagonist. Bioorg. Med. Chem. 12, 3591-3598.

Rathi, L., Kashaw, S.K., Dixit, A., Pandey, G. & Saxena, A.K. (2004). Pharmacophore identification and 3D-QSAR studies in N-(2-benzoyl phenyl)-L- tyrosines as PPAR agonists. Bioorg. Med. Chem. 12, 63-69.

2003

Saxena, A.K., Ram, S., Saxena, M., Singh, N., Prathipati, P., Jain, P.C., Singh, H.K., & Anand, N. (2003). QSAR studies in substituted 1,2,3,4,6,7,12,12a-octahydro-pyrazinop[2',1':6,1]pyrido[3,4-b]indoles- A potent class of neuroleptics. Bioorg. Med.Chem. 11, 2085-2090.

Kashaw, S.K., Rathi, L., Mishra, P. & Saxena, A.K. (2003). Development of 3D-QSAR models in cyclic ureidobenzenesulfonamides: human beta3-adrenergic receptor agonist. Bioorg. Med.Chem. Lett. 13, 2481-2484.

Saxena, A.K. & Prathipati, P. (2003). Comparison of MLR, PLS and GA-MLR in QSAR analysis. SAR and QSAR in Environmental Research, 14, 433-445.

2002

Babu, M.A., Shakya, N., Prathipati, P., Kaskhedikar, S.G. & Saxena, A.K. Development of 3D-QSAR models for 5-Lipoxygenase antagonists: Chalcones. Bioorg. Med.Chem. 10, 4035-4041.

Gupta, N.K., Mishra, P., Prathipati, P. & Saxena, A.K. (2002). 2D- QSAR in hydroxamis acid derivatives as peptide deformylase inhibitors and antibacterial agents. Bioorg. Med.Chem. 10, 3713-3716.

CENTRE FOR CELLULAR & MOLECULAR BIOLOGY, HYDERABAD.

2007

Ganesh, B. & Somdatta, S. (2007). Assortative mixing in Protein Contact Networks and protein folding kinetics. Bioinformatics, 23, 1760-1767.

Maithreye, R. & Somdatta, S. (2007). Propagation of extrinsic perturbation in a negatively auto-regulated pathway. Phys. Biol., 4, 48-59,

Rajesh, S., Sudeshna, S. & Somdata, S. (2007). Synchronization in coupled cells with activator-inhibitor pathways. Phys. Rev. E75, 011906.

Shajahan, T.K., Sinha, S., & Pandit, R. (2007). Cardiac arrhythmias depend sensitively on inhomogeneities in ventricular tissue. Phys.Rev. E75, 011929.

2006

Sridhar, S., Babu, A. V. & Guruprasad, K. (2006). PSSARD (2.0): A database server for making flexible queries relating amino acid sequences to main-chain secondary structure conformations for proteins of known three-dimensional structure and certain useful applications. Int. J. Biol. Macromol. 41, 109-113.

Guruprasad, K., Kartik, V. J., Lavanya, T. & Guruprasad, L. (2006). Juxtaposed half-cystines as disulphide bridged partners in protein tertiary structure. Protein Pept. Lett. 13, 577-579.

Jai, K., V, Lavanya, T. & Guruprasad, K. (2006). Analysis of disulphide bond connectivity patterns in protein tertiary structure. Int. J. Biol. Macromol. 38, 174-179.

Jehan, Z., Vallinayagam, S., Tiwari, S., Pradhan, S., Singh, L., Suresh, A., Reddy, H. M., Ahuja, Y. R. & Jesudasan, R. A. (2006). Novel noncoding RNA from human Y distal heterochromatic block (Yq12) generates testis-specific chimeric CDC2L2. Genome Res. 17, 433-440.

* Amritkar, R.E. & Rangarajan, G. (2006). Spatial synchronization and extinction of species under external forcing. Phys.Rev.Lett. 96, 258102.

2005

Guruprasad, K., Savitha, S. & Babu, A. V. (2005). Computational tools for the analysis of heteroatom groups and their neighbours in protein tertiary structure. Int. J. Biol. Macromol. 37, 35-41.

Guruprasad, K., Srikanth, K. & Babu, A. V. (2005). PSSARD: protein sequence-structure analysis relational database. Int. J. Biol. Macromol. 36, 259-262.

Kotu, A. & Guruprasad, K. (2005). The automatic detection of known beta-propeller structural motifs from protein tertiary structure. Int. J. Biol. Macromol. 36, 176-183.

Bagler, G. & Sinha, S. (2005). Network properties of protein structures. Physica A, 346, 27-33.

Sharadadevi, A., Sivakamasundari, C. & Nagaraj, R. (2005). Amphipathic alpha-helices in proteins: results from analysis of protein structures. Proteins Str. Fn. Bioinf. 59, 791-801.

Thangaraj, K., Chaubey, G., Kivisild, T., Reddy, A.G., Singh, V.K., Rasalkar, A.A. & Singh, L. (2005). Reconstructing the origin of the Andaman islanders. Science, 308, 996.

Thangaraj, K., Chaubey, G., Kivisild, T., Reddy, A.G., Singh, V.K., Rasalkar, A.A. & Singh, L. (2005). Tracing modern human origins. [Response]. Science, 309, 1996-1997.

Suguna, C. & Somdatta, S. (2005). Dynamics of coupled cell-systems. Physica A, 346, 154—164.

2004

* Adindla, S., Guruprasad, K. & Guruprasad, L. (2004). Three-dimensional models and structure analysis of corynemycolyltransferases in Corynebacterium glutamicum and Corynebacterium efficiens. Int. J. Biol. Macromol. 34, 181-189.

Guruprasad, K. & Dhamayanthi, P. (2004). Structural plasticity associated with the beta-propeller architecture. Int. J. Biol. Macromol. 34, 55-61.

* Adindla, S., Inampudi, K. K., Guruprasad, K. & Guruprasad, L. (2004). Identification and analysis of novel tandem repeats in the cell surface proteins of Archaeal and Bacterial genomes using computational tools. Compar. Func. Genom. 5, 2-16.

Basu, M. K. & Mishra, R. K. (2004). Bioinformatics and the art of sequence analysis. Recent adv. in biotech. 24-48.

Sabarinadh, C., Subramanian, S., Tripathi, A. & Mishra, R.K. (2004). Extreme conservation of noncoding DNA near HoxD complex of vertebrates. BMC Genomics, 5, 75.

* Singh, B. K., Rao, J. S., Ramaswamy, R. & Sinha, S. (2004). The role of heterogeneity on the spatiotemporal dynamics of host-parasite metapopulation. Ecolo. Model. 180, 435-443.

Sinha, S. (2004). Multiplicity in non-linear systems. In: Understanding change: models, methodologies and metaphors, Basingstoke, 51-57.

Singh, B. K., Chattopadhyay, J. & Somdatta, S. (2004). The role of virus infection in a simple phytoplankton-zooplankton system. J. Theor. Biol., 231, 153-166.

2003

Guruprasad, K. & Kumari, K. (2003). Three-dimensional models corresponding to the C-terminal domain of human alphaA and alphaB crystallins based on the crystal structure of the small heat-shock protein HSP16.9 from wheat. Int. J. Biol. Macromol. 33, 107-112.

* Guruprasad, K., Rao, M. J., Adindla, S. & Guruprasad, L. (2003). Combinations of turns in proteins. J. Pept. Res. 62, 167-174.

* Guruprasad, K., Shukla, S., Adindla, S. & Guruprasad, L. (2003). Prediction of gamma-turns from amino acid sequences. J. Pept. Res. 61, 243-251.

Guruprasad, K. & Shukla, S. (2003). Prediction of beta-turns from amino acid sequences using the residue-coupled model. J. Pept. Res. 61, 159-162.

Guruprasad, K., Kanagavel, P., Srikanth, K., Radhika, K. & Sonal, S. (2003). Analysis of US patents granted to Indian Inventors. J. Intellectual Property Rights (JIPR), 8, 205-212.

Subramanian, S., Madugula, V. M., George, R., Satishkumar, Pandit, M.W. & Singh, L. (2003). SSRD: simple sequence repeat database for human genome. Comp. Funct. Genomics, 4, 342-245.

Nita, P. & Somdatta, S. (2003). Controllability of Spatiotemporal Systems Using Constant Pinnings. Physica A, 318, 200-212.

2002

Suguna, C. & Somdatta, S. (2002). Cellular Dynamics in Noisy Environment. Fluct. Noise Lett., 2, L313-L326.

Nita, P. & Somdatta, S. (2002). Controlling Dynamics in Spatially Extended Systems. Phys. Rev. E, 65, 0362271 – 0362279.

CENTER FOR DNA FINGERPRINTING AND DIAGNOSTICS, HYDERABAD.

2007

Mudunuri, S. B. & Nagarajaram, H. A. (2007). IMEX: Imperfect Microsatellite Extractor. Bioinformatics (In Press).

* Vidyasagar et. al., (The NMITLI-BioSuite Team) BioSuite: A comprehensive bioinformatics software package (A unique industry academia collaboration). Curr. Sci. 92, 29-38.

Sreenu, V. B., Kumar, P., Nagaraju, J. & Nagarajaram, H. A. (2007). Simple sequence repeats in mycobacterial genomes. J. Biosci. (An invited article in the peer-reviewed special issue on Computational Biology) 32, 1-15.

Sailu, Y., Goyal, K. & Mande, S. C. (2007). Inferring genome-wide functional linkages in prokaryotes by combining improved genome context methods. Genome Res. (In Press).

Ahmed, N., Majeed, A. A., Ahmed, I., Hussain, M. A., Alvi, A., Manjulata, D. S., Rizwan, M., Ranjan, A., Sechi, L. A. & Mégraud, F. (2007). genoBASE pylori, A genotype search tool and database of the human gastric pathogen Helicobacter pylori. Infect. Genet. Evol. (In Press).

Meglecz, E., Anderson, S. J., Bourguet, D., Butcher, R., Caldas, A., Cassel-Lundhagen, A., d'Acier, A. C., Dawson, D. A., Faure, N., Fauvelot, C., Franck, P., Harper, G., Keyghobadi, N., Kluetsch, C., Muthulakshmi, M., Nagaraju, J., Patt, A., Petenian, F., Silvain, J. F. & Wilcock, H. R. (2007). Microsatellite flanking region similarities among different loci within insect species. Insect Mol. Biol. (In press).

Archak, S., Meduri, E., Sravana, K. P. & Nagaraju, J. (2007). InSatDb, A microsatellite database of fully sequenced insect genomes. Nucl. Acids Res. 35, D36 - D39.

2006

Sreenu, V. B., Kumar, P., Nagaraju, J. & Nagarajaram, H. A. (2006). Microsatellite polymorphism across the M. tuberculosis and M. bovis genomes, Implications on genome evolution and plasticity. BMC Genomics, 7, 78.

Achary, M. S., Reddy, A. B., Chakrabarti, S., Panicker, S. G., Mandal, A. K., Ahmed, N., Balasubramanian, D., Hasnain, S. E. & Nagarajaram, H. A. (2006). Disease Causing Mutations in Proteins, Structural Analysis of the CYP1b1 Mutations Causing Primary Congenital Glaucoma in Humans. Biophy. J. 91, 4329-4339.

Goyal, K., Qamra, R. & Mande, S. C. (2006). Multiple gene duplication and rapid evolution in the groEL gene, functional implications. J. Mol. Evol. 63, 781-787.

Vindal, V., Ranjan, S. & Ranjan, A. (2006) In silico Analysis and Classification of Mycobacterium tuberculosis putative GntR transcription regulators. Tuberculosis (In Press).

Ranjan, S., Gundu, R. K. & Ranjan, A. (2006). MycoperonDB, A database of computationally identified operons and transcriptional units in Mycobacteria. BMC Bioinformatics, 7, S5.

Ranjan, S., Seshadri, J., Vindal, V., Yellaboina, S. & Ranjan, A. (2006). iCR, A web tool to identify conserved targets of a regulatory protein across the prokaryotic species. Nucl. Acids Res. 34, W584-W587.

Ranjan, S., Yellaboina, S. & Ranjan, A. (2006). IdeR in mycobacteria, From target recognition to physiological function. Crit. Rev. Microbiol. 32, 69-75.

Yellaboina, S., Ranjan, S., Vindal, V. & Ranjan, A. (2006). Comparative analysis of Iron Regulated genes in mycobacteria. FEBS Lett. 580, 2567-2576.

Bocxlaer, IV, Roelants, K., Biju, S. D., Nagaraju, J. & Bossuyt, F. (2006). Late cretaceous vicariance in gondwanan amphibians. PLoS ONE, 1, e74.

Arunkumar, K. P. & Nagaraju, J. (2006). Unusually long palindromes are abundant in mitochondrial control regions of insects and nematodes. PLoS ONE, 1, e110.

Gandhe, A. S., Arunkumar, K. P., John, S. H. & Nagaraju, J. (2006). Analysis of bacteria-challenged wild silkmoth, Antheraea mylitta (lepidoptera) transcriptome reveals potential immune genes. BMC Genomics, 7, 184.

Archak, S. & Nagaraju, J. (2006). Eicosapentapeptide repeats (EPRs), novel repeat proteins specific to flowering plants. Bioinformatics, 22, 2455-2458.

Arunkumar, K. P., Metta, M. & Nagaraju, J. (2006). Molecular phylogeny of silkmoths reveals the origin of domesticated silkmoth, Bombyx mori from Chinese Bombyx mandarina and paternal inheritance of Antheraea proylei mitochondrial DNA. Mol. Phylogenet. Evol. 40, 419-427.

2005

Cheeran, A., Suganthan, R. B., Swapna, G., Bandey, I., Acharya, S., Nagarajaram, H. A. & Sen, R. (2005). E. coli RNA polymerase mutations located near the upstream edge of RNA,DNA hybrid and the beginning of the RNA exit channel are defective for transcription antitermination by N protein from lambdoid phage H-19B. J. Mol. Biol. 352, 28-43.

Prasad, M. D., Muthulakshmi, M., Arunkumar, K. P., Madhu, M., Sreenu, V. B., Pavithra, V., Bose, B., Nagarajaram, H. A., Mita, K., Shimada, T. & Nagaraju, J. (2005). SilkSatDb, A microsatellite database of the silkworm, Bombyx mori. Nucl. Acids Res. 33, D403-D406.

Prakash, P., Yellaboina, S., Ranjan, A. & Hasnain, S. E. (2005). Computational prediction and experimental verification of novel IdeR binding sites in the upstream sequences of Mycobacterium tuberculosis ORFs. Bioinformatics, 21, 2161-2166.

Prasad, M. D., Muthulakshmi, M., Madhu, M., Archak, S., Mita, K., Nagaraju, J. (2005). Survey and analysis of microsatellites in the silkworm, Bombyx mori, frequency, distribution, mutations, marker potential and their conservation in heterologous species. Genetics, 169, 197-214.

2004

Ahmed, K., Ramesh, G., Srinivas, O., Ramulu, P., Laxman, N., Tasneem, R., Deepak, M., Achary, M. S. & Nagarajaram, H. A. (2004). Design, Synthesis, and Evaluation of Mixed Imine-Amine Pyrrolobenzodiazepine Dimers with Efficient DNA-Binding Affinity and Potent Cytotoxicity. Bioorg. Med. Chem. 12, 5427-5436.

Majeed, A. A., Ahmed, N., Rao, K. R., Ghousunnissa, S., Kausar, F., Bose, B., Nagarajaram, H. A., Katoch, V. M., Cousins, D. V., Sechi, L. A., Gilman, R. H. & Hasnain, S. E. (2004). AmpliBASE MTTM, A Mycobacterium tuberculosis diversity knowledgebase. Bioinformatics, 20,989-992.

Yellaboina, S., Ranjan, S., Chakhaiyar, P., Hasnain, S. E. & Ranjan, A. (2004). Prediction of DtxR regulon, Identification of binding sites and operons controlled by Diphtheria toxin repressor in Corynebacterium diphtheriae. BMC Microbiol. 4, 38.

Yellaboina, S., Seshadri, J., Kumar, M. S. & Ranjan, A. (2004). Predictregulon, A webserver for the prediction of the regulatory protein binding sites and operons in prokaryote genomes Nucl. Acids Res. 32, W318-W320.

2003

Sreenu, V. B. Ranjitkumar, G., Swaminathan, S., Priya, S., Bose, B., Pavan, M. N., Geetha, T., Nagaraju, J. & Nagarajaram, H. A. (2003). MICAS, A fully automated web server for microsatellite extraction and analysis from prokaryote and viral genomic sequences. Appl. Bioinformatics, 2, 165-168.

Ranjit, K., Pavan, G. N., Bose, M., Swaminathan, B., Thanu, S. G., Prashanthi, P. P., Sreenu, V. B. Achary, M. S. & Nagarajaram, H. A. (2003). EMBnet India Node (EIN) at the Centre for DNA Fingerprinting and Diagnostics, Serving the Indian sub-continent in Bioinformatics. Bioinformatics Ind. 2, 67-77.

Sreenu, V. B., Vishwanath, A., Nagaraju, J. & Nagarajaram, H. A. (2003). MICdb, Database of Prokaryotic Microsatellites. Nucl. Acids Res. 31, 106-108.

Yellaboina, S., Chakhaiyar, P., Hasnain, S. E., & Ranjan, A. (2003). Computational prediction of DtxR regulon-A Dissection of physiological process controlled by DtxR in Corynebacterium species. Proceedings of IEEE Computational System Bioinformatics Conference, 442-443.

2002

Kamal, A., Laxman, N., Ramesh, G., Ramulu, P., Srinivas, O., Neelima, K. Kondapi, A. K., Sreenu, V. B. & Nagarajaram H. A. (2002). Design, synthesis, and evaluation of new non-cross linking pyrrolobenzodiazepine dimers with efficient DNA-binding ability and potent antitumour activity J. Med. Chem. 45, 4679-4688.

* Narayanan, E., Nagarajaram, H. A, Ramakrishnan, C. & Srinivasan, N. (2002). Influence of solvent molecules on the stereochemical code of glycine residue. Proteins, 49, 326-334.

Panicker, S. G., Reddy, A.B.M., Mandal, A. K., Ahmed, N., Nagarajaram, H. A., Hasnain, S. E. & Balasubramanian, D. B. (2002). Identification of novel mutations causing familial primary congenital glaucoma in Indian pedigrees. Invest. Ophthalmol. Vis. Sci. 43, 1358-1366.

Qamra, R., Taneja, B. & Mande, S. C. (2002). Identification of conserved residue patterns in small ß-barrel proteins. Prot. Eng. 15, 967- 977.

Prasad, M. D., Nurminsky, D. L. & Nagaraju, J. (2002). Characterization and molecular phylogenetic analysis of mariner elements from wild and domesticated species of silkmoths. Mol. Phylogenet. Evol. 25, 210-217.

CHARAN SINGH UNIVERSITY, MEERUT.

2007
Mohan, A., Goyal, A., Singh, R., Balyan, H. S. & Gupta, P. K. (2007). Physical Mapping of Wheat and Rye Expressed Sequence Tag–Simple Sequence Repeats on Wheat Chromosomes. Crop sci. 47, 3-13.

2005

Singh, R., Kumar, N., Bandopadhyay, R., Rustgi, S., Sharma, S., Balyan, H. S. & Gupta, P. K. (2005). Development and use of anchored-SSRs to study DNA polymorphism in bread wheat (Triticum aestivum L). Mol. Ecol. Notes, 6, 296-299.

2003

Gupta, P. K., Rustgi, S., Sharma, S., Singh, R., Kumar, N. & Balyan, H. S. (2003). Transferable EST-SSR markers for the study of polymorphism and genetic diversity in bread wheat. Mol. Genet. Genomics, 270, 315-323.

DELHI UNIVERSITY, NEW DELHI.

2007

* Singh, S., Samal, A., Giri, V., Krishna, S., Raghuram, N. & Jain, S. (2007). A Universal power law and proportionate change process characterizes the evolution of metabolic networks. Euro. Phys. J. B, 57,75-80.

2006

* Samal, A., Singh, S., Giri, V., Krishna, S., Raghuram, N. & Jain, S.(2006). Low Degree metabolites explain essential reactions and enhance modularity in biological networks. BMC Bioinformatics, 7, 118.

DIRECTORATE OF RICE RESEARCH, HYDERABAD.

2007

Rajendrakumar, P., Biswal, A.K., Balachandran, S.M., Ramesha, M.S., Viraktamath, B.C. & Sundaram, R.M. (2007). A mitochondrial repeat specific marker for distinguishing wild abortive type cytoplasmic male sterile rice lines from their cognate isogenic maintainer lines. Crop sci. 47, 207-211.

Jaikishen, I., Ramesha, M. S., Rajendrakumar, P., Rao, K. S., Neeraja, C. N., Balachandran, S. M., Viraktamath, B. C., Sujatha, K. & Sundaram, R. M. (2007). Characterization of genetic diversity in hybrid rice parental lines using EST-derived and non-EST SSR markers. Rice Genet. Newslett. 23, 24-28.

2006

Rajendrakumar, P., Biswal, A.K., Balachandran, S.M., Srinivasarao, K. & Sundaram, R.M. (2006). Simple sequence repeats in organellar genomes of rice: frequency and distribution in genic and intergenic regions. Bioinformatics, 23, 1-4.

Singh, S.P., Sundaram, R.M., Biradar, S.K., Ahmed, M.I., Viraktamath, B.C. & Siddiq, E.A. (2006). Identification of simple sequence repeat markers for utilizing wide-compatibility genes in inter-subspecific hybrids in rice. Theor. Appl. Genet. 113, 509-517.

GOVIND BALLABH PANT UNIVERSITY, PATNAGAR.

2007

Singh, H., Marla, S. S. & Verma, D. (2007). Comparative Analysis of MMFF94x and AMBER99 force fields using Aspartic Proteases, Serine Proteases, Metallo-Proteases and Sugar-Binding Proteins as different data sets. Online J. Bioinfo. 8, 45-55.

2006

Soma Marla et al, (2006), Comparative Structure and function analysis of chorismate synthase genes in Prevotella rumnicola. Online J. Bioinfo. 7, 35-45.

2005

Naik, P. & Marla, S. (2005). Promoter analysis in E. coli using Positional similarity scoring matrix. Bioinfo. J. 3, 59-63.

INDIAN AGRICULTURAL RESEARCH INSTITUTE, NEW DELHI.

2006

Pathak, H., Wassmann, R., Li, C.R. & Ladha, J.K. (2006). Simulation of Nitrogen Balance in the Rice-Wheat Systems of the Indo-Gangetic Plains. Soil Sci. Soc. Am. J. 70, 1612-1622.

Pathak, H., Singh, R., Bhatia, A. & Jain, N. (2006). Recycling of rice straw to improve Crop yield and soil fertility and reduce atmospheric pollution. Paddy Water Environ. 4, 111-117.

Maiti, D., Das, D. K. & Pathak. H. (2006). Fertilizer requirement for irrigated wheat in eastern India using the QUEFTS simulation model. Sci. World J. 6, 231–245.

Aggarwal, P. K., Kalra, N., Chander, S. & Pathak, H. (2006). InfoCrop: A dynamic Simulation model for the assessment of crop yields, losses due to pests, and environmental impact of agro-ecosystems in tropical environments. I. Model description. Agril. Systems. 89 , 1-25.

Aggarwal, P. K., Banerjee, B., Daryaei, M. G., Bhatia, A., Bala, A., Rani, S., Chander, S.,Pathak, H. & Kalra, N. (2006). InfoCrop: A dynamic simulation model for the assessment of crop yields,

losses due to pests, and environmental impact of agro-ecosystems in tropical environments. II. Performance of the model. Agril. Systems. 89, 47-67.

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE, KOLKOTA.

2005

* Mallick, B., Chakrabarti,J., Satyabrata, S., Ghosh, Z.,& Smarajit, D. (2005). Identity Elements of Archaeal tRNA. DNA Res. 12, 235-246.

* Ghosh, Z., Chakrabarti,J., Mallick, B., Smarajit, D., Satyabrata, S. & Harmeet, S. S. (2005). tRNA-isoleucine-tryptophan Composite Gene .Biochem. Biophys. Res. Comm. 339, 37-40.

Mallick, B., Chakrabarti,J.,Smarajit, D. & Ghosh, Z. (2005). tRNomics: A comparative analysis of Picrophilus torridus with other archaeal thermoacidophiles. Ind. J. biochem. biophys. 42, 238-242.

INDIAN INSTITUTE OF ADVANCED RESEARCH, GUJARAT.

2007

Vijay, S. & Deepak, D. S. (2007). Leishmania major: Genome analysis for identification of putative adhesin-like and other surface proteins. Exp. Parasitol. (In press).

INDIAN INSTITUTE OF CHEMICAL BIOLOGY, KOLKATA.

2006

Bhutoria, S., Mukherjee, P.K., Chhabra, S., Ghoshal, N. (2006). A 3D-QSAR of N- substituted 4-amino3-3-dialkyl-2 (3H)-furanone $GABA_A$ receptor modulators based on Receptor Surface Analysis. Lett. in Drug Desig. Discov. 3, 625-632.

Das, S., Paul, S., Bag, S. K. & Dutta, C. (2006). Analysis of Nanoarchaeum equitans genome and proteome composition: indications for hyperthermophilic and parasitic adaptation. BMC Genomics, 7, 186.

Das, S., Paul, S. & Dutta, C. (2006). Synonymous codon usage in adenoviruses: influence of mutation, selection and protein hydropathy. Virus Res. 117, 227-236.

Das, S., Paul, S. & Dutta, C. (2006). Evolutionary constraints on codon and amino acid usage in two strains of human pathogenic actinobacteria Tropheryma whipplei. J. Mol. Evol. 62, 645-658.

* Ghosh, Z., Chakrabarti, J., Mallick, B., Das, S., Sahoo, S. & Sethi, H. S. (2006). tRNA-isoleucine-tryptophan composite gene. Biochem. Biophys. Res. Commun. 339, 37-40.

Majumder, S., Patra, M. & Mandal, C. (2006). Search for fucose binding domains in recently sequenced hypothetical proteins using molecular modeling techniques and structural analysis. Glycoconj. J. 23, 251-257.

Patra, M., Majumder, S. & Mandal, C. (2006). Structural studies on mannose-selective glycoprotein receptors using molecular modeling techniques. Glycoconj. J. 23, 241-249.

Patra, M. & Mandal, C. (2006). Search for glucose/galactose-binding proteins in newly discovered protein sequences using molecular modeling techniques and structural analysis. Glycobiology, 16, 959-968.

Sharma, P. & Ghoshal, N. (2006). Exploration of a binding mode of benzothiazol-2-yl acetonitrile pyrimidine core based derivatives as potent c-Jun N-terminal kinase-3 inhibitors and 3D-QSAR analyses. J. Chem. Inf. Model. 46, 1763-1774.

2005

Chanda, I., Pan, A. & Dutta, C. (2005). Proteome composition in Plasmodium falciparum: higher usage of GC-rich nonsynonymous codons in highly expressed genes. J. Mol. Evol. 61, 513-523.

Das, S., Ghosh, S., Pan, A. & Dutta, C. (2005). Compositional variation in bacterial genes and proteins with potential expression level. FEBS Lett. 579, 5205-5210.

Das, S., Pan, A., Paul, S. & Dutta, C. (2005). Comparative analyses of codon and amino acid usage in symbiotic island and core genome in nitrogen-fixing symbiotic bacterium Bradyrhizobium japonicum. J. Biomol. Struct. Dyn. 23, 221-232.

Das, S., Paul, S., Chatterjee, S. & Dutta, C. (2005). Codon and amino Acid usage in two major human pathogens of genus bartonella -- optimization between replicational-transcriptional selection, translational control and cost minimization. DNA Res. 12, 91-102.

* Mallick, B., Chakrabarti, J., Sahoo, S., Ghosh, Z. & Das, S. (2005). Identity Elements of Archaeal tRNA. DNA Res. 12, 235-246.

2004

Ghoshal, N. & Mukherjee, P. K. (2004). 3-D-QSAR of N-substituted 4-amino-3,3-dialkyl-2(3H)-furanone GABA receptor modulators using molecular field analysis and receptor surface modelling study. Bioorg. Med. Chem. Lett. 14, 103-109.

Majumder, S., Roy, A. & Mandal, C. (2004). Prediction of 3-D structures of fucose-binding proteins and structural analysis of their interaction with ligands. Glycoconj. J. 20, 545-550.

Mukhopadhyay, A., Talukdar, S., Bhattacharjee, A. & Ray, K. (2004). Bioinformatic approaches for identification and characterization of olfactomedin related genes with a potential role in pathogenesis of ocular disorders. Mol. Vis. 10, 304-314.

2003

Chattopadhyay, S. & Chakrabarti, J. (2003). Temporal changes in phosphoglycerate kinase coding sequences: a quantitative measure. J. Comput. Biol. 10, 83-93.

Chattopadhyay, S., Sahoo,S., Kanner, W.A. & Chakrabarti, J. (2003). Pressures in Archaeal Protein Coding Genes:A Comparative Study. Compar. Funct. Genom. 4, 56-65.

Mukherjee, S., Mukhopadhyay, A., Chaudhuri, K. & Ray, K. (2003). Analysis of haemophilia B database and strategies for identification of common point mutations in the factor IX gene. Haemophilia, 9, 187-192.

Som, A., Sahoo, S., Mukhopadhyay, I., Chakrabarti, J. & Chaudhury, R. (2003). Scaling violations in coding DNA. Europhys. Lett. 62, 271-277.

2002

Chattopadhyay, S., Kanner, W.A. & Chakrabarti, J. (2002). DNA nucleotides: A case study of evolution. Eur. Phys. J. B 26, 393-398.

Mukhopadhyay, A., Gupta, A., Mukherjee, S., Chaudhuri, K. & Ray, K. (2002). Did myocilin evolve from two different primordial proteins? Mol. Vis. 8, 271-279.

INDIAN INSTITUTE OF CHEMICAL TECHNOLOGY, HYDERABAD.

2006

Murty, U. S. N., Rao. M. S., Neelima, A. & Krishna, A. R. (2006). Database management system for control of malaria in Arunachal Pradesh, India. Bioinformation, 1, 194-196.

2005

Praveen, B., Vincent, S., Murty, U. S. N., Krishna, A. R. & Jamil, K. (2005). Rapid identification system for Metallothionine proteins using Expert System. Bioinformation, 1, 14-15.

Kumar, D. V. R. S., Sriram, K., Madhusudhan R. K. & Murty, U. S. N. (2005). Management of filariasis using prediction rules derived from data mining. Bioinformation, 1, 8-11.

Murty, U. S. N., Kumar, D. V. R. S., Sriram, K., Madhusudhan, R. K. K. Bhattacharyulu, C. H. N. V., Praveen, B. & Radha Krishna, A. (2005). A Web based relational database management system for filariasis control. Bioinformation, 1, 19-20.

Rayavarapu, B., Siddharth, V. & Upadhyayula S. M. (2005). Modeling analysis of GST (glutathione-S-transferases) from Wuchereria bancrofti and Brugia malayi. Bioinformation, 1, 25-27.

Bhargavi, R., Sastry, G. M., Murty, U. S. N. & Sastry, G. N. (2005). Structural and active site analysis of plasmepsins of Plasmodium falciparum: Potential anti-malarial targets. Int. J. Biol. Macromol. 37, 73-84.

2004

Bindu, P. H., Sastry, G. M., Murty, U. S. N. & Sastry, G. N. (2004). Structural and conformational changes concomitant with the E1-E2 transition in H(+)K(+)-ATPase: a comparative protein modeling study. Biochem. Biophys. Res. Commun. 319, 312-320.

2002

Sharma, D. C. (2002). Software forecasts tropical diseases. Lancet Infect. Dis. 2, 66.

Murty, U. S. N. (2002). Database on Filariasis, (Websites of interest). Trends in Parasitol. 18, 436.

INDIAN INSTITUTE OF SCIENCE, BANGALORE.

2007

Vetriselvi, R. & Bansal, M. (2007). Identification and annotation of promoter regions in microbial genome sequences on the basis of DNA stability. J. Biosci. 32.

Mondal, S., Mohan, B. R., Bhavna, R. & Ramakumar, S. (2007). In silico detection of binding mode of J-superfamily conotoxin pl14a with Kv1.6 channel. In Silico Biol. 7, 0018.

* Gowri, B. A. S., Sarani, R., Daliah, M., Mridula, P., Vasuki, C. R., Sowmiya, G., Vasundhar, B., Sudha, P., Jeyakanthan, J., Velmurugan, D. & Sekar, K. (2007). Ion-pairs in non-redundant protein structures. J. Biosci. 32, 693-704.

Balamurugan, B., Roshan, M.N.A.Md., Shaahul, H. B., Sumathi, K., Senthilkumar, R., Udayakumar, A., Venkatesh, B. K. H., Kalaivani, M., Sowmiya, G., Sivasankari, P., Saravanan, S., Vasuki, R. C., Gopalakrishnan, K., Selvakumar, K. N., Jaikumar, M., Brindha, T., Daliah, M. and Sekar, K. (2007). PSAP : Protein Structure Analysis Package. J. Appl. Cryst. 40, 773-777.

Srinivasan, N., Sowdhamini, R. & Bhattacharya, A. (2007). Computational Biology: More than just a set of techniques. J. Biosci. 32, 1-2.

Balaji, S. & Srinivasan, N. (2007). Comparison of sequence-based and structure-based phylogenetic trees of homologous proteins: Inferences on protein evolution. J. Biosci. 32, 83-96.

Vani, J., Jeyakani, J., Chandra, N. R., Nayak, R. & Shaila, M. S. (2007). Peptidomimics of antigen are present in variable region of heavy and light chains of anti-idiotypic antibody and function as surrogate antigen for perpetuation of immunological memory. Mol. Immunol. 44, 3345-3354.

Prashanth, K., Prabhu, R., Chandra, N. R., Soumyendu, R. & Govindarajan, R. (2007). Parallel Implementation of Autodock. J. Appl. Cryst. 40, 598-599.

Prashant, K., Samta, M., Nirmal, K., Sriram, I. M., Balakrishnan, N. & Chandra, N. R. (2007). Cytoview: Development of a Cell modeling framework. J. Biosci. 32.

Konkimalla, V. B., Suhas, V. L., Chandra, N. R., Gebhart, E. & Efferth, T. (2007). Diagnosis and therapy of oral squamous cell carcinoma. Expert Rev. Anticancer Ther. 7, 317-329.

* Vidyasagar, Chandra N. R., Vishveshwara, S. et al., (NMITLI consortium for BioSuite). (2007). BioSuite: A comprehensive bioinformatics software package (a unique-industry- academia collaboration). Curr. Sci. 92, 29-38.

Bhattacharya, S., Bhattacharya, C. & Chandra, N. R. (2007). Comparison of protein structures by growing neighborhood alignments. BMC Bioinformatics, 8, 77.

Kim, S.M., Bowers, P.M., Pal, D., Strong, M., Terwilliger, T.C., Kaufmann,M. & Eisenberg, D. (2007). Functional linkages reveal protein complexes for structure determination. Structure (In press).

Padmashri, S. K. & Sikdar, S. K. (2007). Glutamate pretreatment affects Ca (2+) signaling in processes of astrocyte pairs. J. Neurochem. 100, 105-117.

Hariharan, N., Ding, M. & Rangarajan, G. (2007). Mitigating the effects of measurement noise on Granger causality. Phys. Rev. E75, 031123:1-10.

Verkhedkar, K., Raman, K., Chandra, N. & Vishveshwara S. (2007). Metabolome based reaction graphs of M. tuberculosis and M. leprae: A comparative network analysis. PLoS ONE (In Press).

Kanade, S. R., Suhas, V. L., Chandra N. & Gowda L. R. (2007). Functional interaction of diphenols with polyphenol oxidase. FEBS J. 274, 4177-87.

Singh, D. D., Chandran, D., Jeyakani, J. & Chandra, N. (2007). Scanning the Genome of Mycobacterium Tuberculosis to Identify Potential Lectins. Protein. Pept. Lett. (In Press).

Sivapriya, K., Hariharaputran, S., Suhas, V. L., Chandra, N. & Chandrasekaran, S. (2007). Conformationally locked thiosugars as potent alpha-mannosidase inhibitors: Synthesis, biochemical and docking studies. Bioorg. Med. Chem. 15, 5659-5665.

Dash, B. P., Mukherjee, S., Suhas, V. L. & Chandra N. (2007). Interaction Profiling of T-Cell Epitopes with MHC-Class I Molecules. Protein Pept Lett. 14, 557-564.

Raman, K., Rajagopalan, P. & Chandra, N. (2007). Hallmarks of Mycolic acid Biosynthesis: A comparative genomics study. Proteins. (In Press).

Vani, J., Jeyakani, J., Chandra, N. R., Nayak, R. & Shaila, M. S. (2007). Peptidomimetics of antigen are present in variable region of heavy and light chains of anti-idiotypic antibody and function as surrogate antigens for perpetuation of immunological memory. Mol. Immunol. 44, 3345-3354.

Sriharsha, S. N., Pai, K. S. R., Suhas, V. L., Shashikanth, S. & Chandra, N. R. (2007). Synthesis, Docking and anti-tumor activity of β-L-1,3-Thiazolidine pyrimidine nucleoside analogues. Curr. Med. Chem. (In Press).

Krishna, R., Prabu, J. R., Manjunath, G. P., Datta, S., Chandra, N. R., Muniyappa, K. & Vijayan, M. (2007). Snapshots of RecA protein involving movement of the C-domain and different conformations of the DNA-binding loops: crystallographic and comparative analysis of 11 structures of Mycobacterium smegmatis RecA. J. Mol. Biol. 367, 1130-1144.

2006

Kundhavai, N. S., Srinivas, O., Nivedita, M., Sagarika, D., Jayaraman, N., Surolia, A. & Vijayan, M. (2006). Multivalency in lectins. A crystallographic, modelling and light scattering study involving peanut lectin and a bivalent ligand. Curr. Sci. 90, 1230-1237.

Sathyapriya, R., Brinda, K. V. & Vishveshwara, S. (2006).Correlation of the Side-Chain Hubs with the Functional Residues in DNA Binding Protein Structures. J. Chem. Inf. Model. 46, 123-129.

Priti, H., Vishveshwara, S. & Samir, K. P. (2006). Tryptophan-water interaction in Monellin: Hydration patterns from molecular dynamics simulation. Chem. Phys. Lett. 420, 517-522.

Priti, H., Guruprasad, N. & Vishveshwara, S. (2006). Ab initio studies on the tri- and diphosphate fragments of adenosine triphosphate. Biophys. Chem. 119, 127-136.

Brinda, K.V. & Vishveshwara, S. (2006). Characterization of the backbone geometry of protein native state structures. Proteins Str. Fn. Bioinf. 64, 992-1000.

* Mukherjee, S., Bansal, M & Bhattacharyya, D. (2006). Conformational Specificity of Non-Canonical Base Pairs and Higher Order Structures in Nucleic Acids: Crystal Structure Database Analysis. J. Comp. Aided Mol. Des. 20, 629-645.

Mondal, S., Bhavna, R., Mohan, B. R. & Ramakumar, S. (2006). Pseudo amino acid composition and multi-class support vector machines approach for conotoxin superfamily classification. J. Theor. Biol. 243, 252-260.

Mondal, S., Babu, R. M., Bhavna, R. & Ramakumar, S. (2006). I-conotoxin superfamily revisited. J. Pept. Sci. 12, 679-685.

Manikandan, K., Bhardwaj, A., Guptam, N., Lokanath, N. K., Ghosh, A., Reddy, V. S. & Ramakumar, S. (2006). Crystal structures of native and xylosaccharide-bound alkali thermostable xylanase from an alkalophilic Bacillus sp. NG-27: structural insights into alkalophilicity and implications for adaptation to polyextreme conditions. Protein Sci. 15, 1951-1960.

Bagaria, A., Surendranath, K., Ramagopal, U. A., Ramakumar, S. & Karande, A. A. (2006). Structure-function analysis and insights into the reduced toxicity of Abrus precatorius agglutinin I in relation to abrin. J. Biol. Chem. 281, 34465-34474.

Padyana, A. K. & Ramakumar, S. (2006). Lateral energy transfer model for adjacent light-harvesting antennae rods of C-phycocyanins. Biochim. Biophys. Acta. 757, 161-165.

Balamurugan, B., Roshan, M. N. A. Md., Daliah, M., Ambaree, M., Divya, S., Keerthana, H., Seemanthini, M. & Sekar, K. (2006). SMS: Sequence, Motif and Structure – A database on the structural rigidity of peptide fragments in non-redundant proteins. In Silico Biol. 6, 229-235.

Sumathi, K., Ananthalakshmi, P., Roshan, M. N. A. Md. & Sekar, K. (2006). 3dSS: 3-Dimensional Structural Superposition. Nucl. Acids Res. 34, W128-W134.

* Jeyalakshmi, J., Vaijayanthimala, S., Velmurugan, D., Mridula, P. & Sekar, K. (2006). Interaction of water molecules in non-identical protein structures. Ind. J. Chem. 45, 159-162.

Thathoo, R., Virmani, A., Sai, S. L., Balakrishnan, N. & Sekar, K. (2006). TVSBS: A fast exact pattern matching algorithm for biological sequences. Curr. Sci. 91, 47-53.

Guruprasad, S. & Sekar, K. (2006). Artificial life and living systems: Insight into artificial Life and its implications in life science research. Bioinformation, 1, 139-140.

Mahesha, H. G., Singh, S. A., Srinivasan, N. & Rao, A. G. A. (2006). A spectroscopic study of the interactions of isoflavones with human serum albumin. FEBS J. 273, 451-467.

Gowri, V. S., Krishnadev, O., Swamy, C. S. & Srinivasan, N. (2006). MulPSSM: A database of multiple position specific scoring matrices of protein domain families. Nucl. Acids Res. 34, D243-246.

Srinivasan, N. (2006). Computational Biology and Bioinformatics: A tinge of Indian spice. Bioinformation, 1, 105-109.

* Bhadra, R., Sandhya, S., Abhinandan, K. R., Chakrabarti, S., Sowdhamini, R. & Srinivasan, N. (2006). Cascade PSI-BLAST Web server: A remote homology search tool for relating protein domains. Nucl. Acids Res. 34, W143-W146.

Tyagi, M., Sharma, P., Swamy, S., Cadet, F., Srinivasan, N., de Brevern, A. G. & Offmann, B. (2006). Protein Block Expert (PBE): A web-based protein structure analysis server using a structural alphabet. Nucl. Acids Res. 34, W119-W223.

* Pugalenthi, G., Shameer, K., Srinivasan, N. & Sowdhamini, R. (2006). HARMONY: a web-server for the assessment of protein structures. Nucl. Acids Res. 34, W231-W234.

Krupa, A., Anamika & Srinivasan, N. (2006). Genome wide comparative analyses of domain organisation of repertoires of protein kinases of Arabidopsis thaliana and Oryza sativa. Gene, 318, 1-13.

Tyagi, M., Gowri, V. S., Srinivasan, N., de Brevern, A. G. & Offmann, B. (2006). A substitution matrix for structural alphabet based on structural alignment of homologous proteins and its

applications. Proteins Str. Fn. Bioinf. 65, 32-39.

Sharma, K., Gupta, M., Krupa, A., Srinivasan, N. & Singh, Y. (2006). EmbR, a regulatory protein with ATPase activity, is a substrate of multiple serine/threonine kinases and phosphatase in Mycobacterium tuberculosis. FEBS J. 273, 2711-2721.

Gowri, V. S., Tina K. G., Krishnadev, O. & Srinivasan, N. (2006). Strategies for the effective identification of remotely related sequences in multiple PSSM search approach. Proteins Str. Fn. Bioinf. 67, 789-794.

Thangudu, R. R., Sharma, P., Srinivasan, N. & Offmann, B. (2006). Analycys: a database for conservation and conformation of disulphide bonds in homologous proteins. Proteins Str. Fn. Bioinf. 67, 255-261.

Talla, V., Narayanan, C., Srinivasan, N. & Balasubramanian, D. (2006). Mutations causing self-aggregation in human γC crystalline leads to congenital cataract. Invest. Ophthalmol. Vis. Sci. 47, 5212-5217.

Ramesha, K. P., Gowda, S., Chandra, N. R. & Rao, M. R. S. (2006). Single nucleotide polymorphisms in α-lactalbumin gene in cattle and their effect on the mature protein. Indian J. Anim. Sci. 76, 816-820.

Bhavani, S., Nagargadde, A., Thawani, A., Sridhar, V. & Chandra, N. R. (2006). Substructure-Based Support Vector Machine Classifiers for Prediction of Adverse Effects in Diverse Classes of Drugs. J. Chem. Inf. Model, 46, 2478 -2486.

Ramesh, S., Bharath, M. M., Chandra, N. R., Rao, M. R. (2006). A K52Q substitution in the globular domain of histone H1t modulates its nucleosome binding properties. FEBS Lett. 580, 5999-6006.

Vinod, P. K., Konkimalla, B., Chandra, N. R. (2006). In-silico pharmacodynamics: correlation of adverse effects of H2-antihistamines with histamine N-methyl transferase binding potential. Appl Bioinformatics, 5, 141-150.

Chandra, N. R. (2006). Common scaffolds, diverse recognition profiles. Structure. 14, 1093-1094.

Chandra, N. R., Kumar, N., Jeyakani, J., Singh, D. D., Gowda, S. B., Prathima, M. N. (2006). Lectindb: a plant lectin database. Glycobiology, 16, 938-946.

Karthik, R., Preethi, R. & Chandra, N. R. (2006). Principles and Practices of Pathway modeling. Curr. Bioinformatics, 1, 147-160.

Rajan, P., Vetriselvi, R. & Chandra, N. R. (2006). Carbohydrate based drug design: Recognition fingerprints and their use in lead identification. Indian J. Chem. 45, 77-92.

Vani, J., Shaila, M. S., Chandra, N. R. & Nayak, R. (2006). A combined immuno-informatics and structure-based modeling approach for prediction of T cell epitopes of secretory proteins of Mycobacterium tuberculosis. Microbes Infect. 8, 738-746.

Bhattacharya, S., Bhattacharya, C. & Chandra, N. R. (2006). Projections for fast protein structure retrieval. BMC Bioinformatics, 7, S5.

Rao, S. P. & Sikdar, S. K. (2006). Astrocytes in 17β-estradiol treated mixed hippocampal cultures show attenuated calcium response to neuronal activity. Glia, 53, 817-826.

Majumdar, S. & Sikdar, S. K. (2006). G-protein activation modulates pseudo-periodic oscillation of Na channel. Biochem. Biophys. Res. Commun. 347, 444-451.

* Amritkar, R. E. & Rangarajan, G. (2006). Spatial synchronization and extinction of species under external forcing. Phys. Rev. Lett. 96, 258102.

2005

Sung K. K., Ananthasuresh, G. K. & Vishveshwara, S. (2005). A Deterministic Optimization Approach to Protein Sequence Design Using Continuous Models. The Int. J. Robot. Res. 24, 109-130.

Sathyapriya, R. & Vishveshwara, S. (2005). Short hydrogen bonds in proteins. FEBS J. 272,1819-1832.

Brinda, K. V. & Vishveshwara, S. (2005). A Network Representation of Protein Structures: Implications for Protein Stability. Biophy. J. 89, 4159-4170.

Brinda, K. V. & Vishveshwara, S. (2005). Oligomeric protein structure networks: Insights into protein-protein interactions. BMC Bioinformatics, 6, 296.

Sistla, R. K., Brinda, K. V. & Vishveshwara, S. (2005). Identification of Domains and Domain Interface Residues in Multidomain Proteins from Graph Spectral Method. Proteins Str. Fn. Bioinf. 59, 616-626.

Brinda, K. V., Surolia, A. & Vishveshwara, S. (2005). Insights into the quaternary association of proteins through structure graphs: A case study of lectins. Biochem. J. 391, 1-15.

Krishnadev, O., Brinda, K. V. & Vishveshwara, S. (2005). A Graph Spectral Analysis of the Structural Similarity Network of Protein Chains. Proteins Str. Fn. Bioinf. 61, 152-163.

Sanjeev, B. S. & Vishveshwara, S. (2005). Dynamics of the native and the ligand-bound structures of eosinophil cationic protein: Network of hydrogen bonds at the catalytic site. J. Biomol. Struct. Dyn. 22, 657-671.

Kanhere, A. & Bansal, M. (2005). A novel method for prokaryotic promoter prediction based on DNA stability. BMC Bioinformatics, 6, 1.

Madhumalar, A. & Bansal, M. (2005). Sequence preference for BI/BII conformations in DNA: MD and crystal structure data analysis. J. Biomol. Struct. Dyn. 23, 13-27.

Kanhere, A. & Bansal, M. (2005). Structural properties of promoters: similarities and differences between prokaryotes and eukaryotes. Nucl. Acids Res. 33, 3165-3175.

Bhattacharjee, A. & Bansal, M. (2005). Collagen Structure: The Madras triple helix and the current scenario. IUBMB Life, 57, 161-172.

Mondal, S., Vijayan, R., Shichina, K., Babu, R. M. & Ramakumar, S. (2005). I-superfamily conotoxins: sequence and structure analysis. In Silico Biol. 5, 557-571.

* Gupta, K., Thomas, D., Vidya, S. V., Venkatesh, K. V. & Ramakumar, S. (2005). Detailed protein sequence alignment based on Spectral Similarity Score (SSS). BMC Bioinformatics, 6, 105.

Balamurugan, B., Samaya, K. M., Ramesh, J., Roshan, M. N. A. Md., Sumathi, K. & Sekar, K. (2005). SSEP - 2.0: Secondary Structural Elements of Proteins. Acta Cryst. D61, 634-636.

Ananthalakshmi, P., Samaya, K. M., Chockalingam, C., Mayilarasi, C. & Sekar, K. (2005). PDB Sequence Search Tool (PSST 2.0). Appl. Bioinformatics, 4, 141-145.

Samaya, K. M., Sheik, S. S., Ramesh, J., Balamurugan, B., Jeyasimhan, M., Mayilarasi, C. & Sekar, K. (2005). CADB - 2.0: Conformation Angles DataBase. Acta Cryst. D61, 637-639.

Ananthalakshmi, P., Kiran, Ch. K., Jeyasimhan, M., Sumathi, K. & Sekar, K. (2005). FF - Fragment Finder: A web based software to identify similar three-dimensional structural motif. Nucl. Acids Res. 33, W85-W88.

Sheik, S. S., Aggarwal, S. K., Poddar, A., Sathiyabhama, B., Balakrishnan, N. & Sekar, K. (2005). Analysis of string searching algorithms on biological sequence databases. Curr. Sci. 89, 368-374.

Anamika, Srinivasan, N. & Krupa, A. (2005). A genomic perspective of protein kinases in Plasmodium falciparum. Proteins Str. Fn. Bioinf. 58, 180-189.

* Rekha, N., Machado, S. M., Narayanan, C., Krupa, A. & Srinivasan, N. (2005). Interaction interfaces of protein domains are not topologically equivalent across families within superfamilies: Implications for metabolic and signalling pathways. Proteins Str. Fn. Bioinf. 58, 339-353.

Gadkari, R., Roy, S., Murthy, G. S., Rekha, N., Srinivasan, N. & Dighe, R. R. (2005). Identification Of A Heterodimer-Specific Epitope Present In Human Chorionic Gonadotropin (hCG) Using A Monoclonal Antibody That Can Distinguish Between hCG and Human Luteinizing Hormone. J. Mol. Endocrin. 34, 879-884.

Anand, B., Gowri, V. S. & Srinivasan, N. (2005). Use of multiple profiles corresponding to a sequence alignment enables effective detection of remote homologues. Bioinformatics, 21, 2821-2826.

Krishnadev, O., Rekha, N., Pandit, S. B., Abhiman, S. S., Mohanty, Swapna, L.S., Gore, S. & Srinivasan, N. (2005). PRODOC resource for comparison of tethered protein domain architectures with in-built information on distantly related domain families. Nucl. Acids Res. 33, W126-W129.

Bhadra, R., Srinivasan, N. & Pandit, S. B. (2005). A new domain family in the superfamily of alkaline phosphatases. In Silico Biol. 5, 379-387.

* Sandhya, S., Chakrabarti, S., Abhinandan, K. R., Sowdhamini, R. & Srinivasan, N. (2005). Assessment of a rigorous transitive profile based search method to detect remotely similar proteins. J. Biomol. Struct. Dyn. 23, 283-298.

De, S., Krishnadev, O., Srinivasan, N. & Rekha, N. (2005). Interaction preferences across protein-protein interfaces of obligatory and non-obligatory components are different. BMC Struct. Biol. 5, 15.

Krupa, A. & Srinivasan, N. (2005). Diversity in domain architectures of Ser/Thr kinases and their homologues in prokaryotes. BMC Genomics, 6, 129.

Padmanabhan, P. K., Mukherjee, A., Singh, S., Chattopadhyaya, S., Gowri, V. S., Myler, P. J., Srinivasan, N. & Rentala, M. (2005). Glyoxalase I from Leishmania donovani: A potential target for anti-parasite drug. Biochem. Biophys. Res. Commun. 337, 1237-1248.

Raman, K., Rajagopalan, P. & Chandra, N. R. (2005). Flux balance analysis of mycolic Acid pathway: targets for anti-tubercular drugs. PLoS Comput. Biol. 1, e46.

Chaitra, M. G, Hariharaputran, S., Chandra, N. R., Shaila, M. S. & Nayak, R. (2005). Defining putative T cell epitopes from PE and PPE families of proteins of Mycobacterium tuberculosis with vaccine potential. Vaccine, 23, 1265-1272.

Pal, D. & Eisenberg, D. (2005). Inference of protein function from protein structure. Structure, 13, 121-30.

Bedathur, S. & Haritsa, J. (2005). Search-Optimized Suffix-tree Storage for Biological Applications. Proc. of 12th IEEE Intl. Conf. on High Performance Computing (HiPC), 29-39.

Majumdar, S. & Sikdar, S. K. (2005) Fast pseudo-periodic oscillations in the rat brain voltage-gated sodium channel a subunit. J. Memb. Biol. 208, 1-14.

2004

Sanjeev, B. S. & Vishveshwara, S. (2004). Protein-Water Interactions in Ribonuclease A and Angiogenin: A Molecular Dynamics Study. Proteins Str. Fn. Bioinf. 55, 915-923.

Kalyan, S. C., Sanjeev, B. S. & Vishveshwara, S. (2004). Stability and Dynamics of the Domain Swapped Bovine-Seminal Ribonuclease. Chem. Biodivers. 1, 802-818.

Sanjeev, B. S. & Vishveshwara, S. (2004). Conformational Transitions in Eosinophil Cationic Protein: A Molecular Dynamics Study in Aqueous Environment. J. Biomol. Struct. Dyn. 22, 171-182.

Brinda, K.V., Nivedita, M., Surolia, A. & Vishveshwara, S. (2004). Determinants of quaternary association in legume lectins. Protein Sci. 13, 1735-1749.

Sathyapriya, R. & Vishveshwara, S. (2004). Interaction of DNA with Clusters of Amino acids in Proteins. Nucl. Acid Res. 32, 4109-4118.

* Kanhere, A. & Bansal, M. (2004). DNA Bending and Curvature: A Turning Point in DNA Function. Proc. Indian Natl. Sci. Acad. B70, 239-254.

Mathur, P., Ramakumar, S. & Chauhan, V. S. (2004). Peptide design using alpha,beta-dehydro amino acids: from beta-turns to helical hairpins. Biopolymers, 76, 150-161.

Rudresh, Ramakumar, S., Ramagopal, U. A., Inai, Y., Goel, S., Sahal, D. & Chauhan, V. S. (2004). De novo design and characterization of a helical hairpin eicosapeptide; emergence of an anion receptor in the linker region. Structure, 12, 389-396.

* Fernando, S. A., Selvarani, P., Das, S., Kumar, ChK., Mondal, S., Ramakumar, S. & Sekar, K. (2004). THGS: a web-based database of Transmembrane Helices in Genome Sequences. Nucl. Acids Res. 32, D125-D128.

Manikandan, K. & Ramakumar, S. (2004). The occurrence of C--H...O hydrogen bonds in alpha-helices and helix termini in globular proteins. Proteins, 56, 768-781.

Pidugu, L. S., Kapoor, M., Surolia, N., Surolia, A. & Suguna, K. (2004). Structural basis for the variation in triclosan affinity to enoyl reductases. J. Mol. Biol. 343, 147-155.

Samaya, K. M., Soma, D., Chockalingam, C., Shanthi, V. & Sekar, K. (2004). LySDB: Lysozyme Structural Database. Acta Cryst. D60, 597-600.

Selvarani, P., Shanthi, V., Rajesh, C. K., Saravanan, S. & Sekar, K. (2004). BSDD: Biomolecules Segment Display Device - A web based interactive display tool. Nucl. Acids Res. 32, W645-W648.

* Fernando, S. A., Selvarani, P., Soma, D., Kiran, Ch. K., Sukanta, M., Ramakumar, S. & Sekar, K. (2004). THGS: A web based database of Transmembrane Helices in Genome Sequences. Nucl. Acids Res. 32, D125-D128.

Sheik, S. S., Agarwal, S. K., Poddar, A., Balakrishnan, N. & Sekar, K. (2004). A Fast Pattern Matching Algorithm. J. Chem. Inf. Comp. Sci. 44, 1251-1256.

Krupa, A., Abhinandan, K. R. & Srinivasan, N. (2004). KinG: A database of protein Kinases IN Genomes. Nucl. Acids Res. 32, 153-155.

Singh, S., Rekha, N., Pillai, B., Singh, V., Naorem, A., Sampath, V., Srinivasan, N. & Sadhale, P. P. (2004). Domainal Organization Of The Lower Eukaryotic Homologs Of The Yeast RNA Polymerase II Core Subunit Rpb7 Reflects Functional Conservation. Nucl. Acids Res. 32, 201-210.

Rahaman, A., Srinivasan, N., Shamala, N. & Shaila, M. S. (2004). Phosphoprotein of Rinderpest virus forms a tetramer through coiled-coil region important for biological function: A structural insight. J. Biol. Chem. 279, 23606-23614.

Anand, B., Namboori, S., Sandhya, S. & Srinivasan, N. (2004). Influence of protein structural similarities in adding value to genome data. Ind. J. Biotech. 3, 473-485.

Pandit, S. B., Bhadra, R., Gowri, V. S., Balaji, S., Anand, B. & Srinivasan, N. (2004). SUPFAM: A database of sequence superfamilies of protein domains. BMC Bioinformatics, 5, 28.1-28.5.

Krupa, A., Preethi, G. & Srinivasan, N. (2004). Structural modes of stabilization of permissive phosphorylation sites in protein kinases: Distinct strategies in Ser/Thr and Tyr kinases. J. Mol. Biol. 339, 1025-1039.

Mahajan, A., Sharma, A., Chavali, S., Kabra, M., Chowdhury, M. R., Srinivasan, N. & Bharadwaj, D. (2004). Novel missense mutation in the coagulation factor IX catalytic domain associated with severe hemophilia B factor IX$_{Delhi}$. Haemophilia, 10, 550-552.

Namboori, S., Mhatre, N., Sujatha, S., Srinivasan, N. & Pandit, S. B. (2004). Enhanced functional and structural domain assignments using remote similarity detection procedures for proteins encoded in the genome of Mycobacterium tuberculosis H37Rv. J. Biosci. 29, 245-259.

Namboori, S., Srinivasan, N. & Pandit, S. B. (2004). Recognition of remotely related structural homologues using sequence profiles of aligned homologous protein structures. In Silico Biol. 4, 445-460.

Pandit, S. B., Balaji, S. & Srinivasan, N. (2004). Structural and functional characterization of gene products encoded in the human genome by homology detection. IUBMB Life, 56, 317-331.

Pandit, S. B. & Srinivasan, N. (2004). Identification and analysis of a new family of bacterial serine proteinases. In Silico Biol. 4, 563-572.

Tejasvini, P., Tamilselvi, S., Sridhar, H., Chaitra, H. S. & Chandra, N. (2004). Extracting Hydrogen-Bond Signature Patterns From Protein Structure Data. J. Appl. Bioinformatics, 3, 125-135.

Raval, S., Gowda, S. B., Singh, D. D. & Chandra, N. R. (2004). A database analysis of 'jacalin-like' lectins: sequence-structure-function relationships. Glycobiology, 14, 1247-1263.

Kumar, P., Rao, A. G., Hariharaputran, S., Chandra, N. & Gowda, L. R. (2004). Molecular mechanism of dimerizationof bowman-birk inhibitors: Pivotal role of ASP76 in dimerization. J. Biol. Chem. 279, 30425-30432.

Shanmugham, D., Chandra, N. R., Chandrasekhar, S. B. K., Rangarajan, P. N. & Govindarajan, P. (2004). d-aminolevulinate dehydrase from plasmodium falciparum - indigenous vs imported. J. Biol. chem. 279, 6934-6942.

* Bhattacharyya, R., Pal, D. & Chakrabarti, P. (2004). Disulfide bonds, their stereospecific environment and conservation in protein structures. Protein Eng. Des. Sel. 17, 795-808.

Bhattacharyya, C., Grate, L. R., Jordan, M. I., El Ghaoui, L. & Mian, I. S. (2004). Robust sparse hyperplane classifiers: application to uncertain molecular profiling data. J. Comput. Biol. 11, 1073-1089.

Bedathur, S. & Haritsa, J. (2004). Engineering a Fast Online Persistent Suffix Tree Construction. Proc. of 20th IEEE Intl. Conf. on Data Engineering (ICDE), 720-731.

Neelapala, N., Mittal, R. & Haritsa, J. (2004). SPINE: Putting Backbone into String Indexing. Proc. of 20th IEEE Intl. Conf. on Data Engineering (ICDE), 325-336.

Bedathur, S., Kadlag, A. & Haritsa, J. (2004). BODHI: A Database Habitat for Bio-diversity Information. Proc. of ACM SIGMOD Intl. Conf. on Management of Data, 953-954.

Majumdar, S., Foster, G. & Sikdar, S. K. (2004). Induction of pseudo-periodic oscillation in voltage-gated sodium channel properties is dependent on the duration of prolonged depolarization. Eur. J. Neurosci. 2O, 127-143.

Albo, Z., Di Prisco, G. V., Chen, Y., Rangarajan, G., Truccolo, W., Feng, J., Vertes, R. P. & Ding, M. (2004). Is partial coherence a viable technique for identifying generators of neural oscillations? Biol. Cybernet. 9O, 318-326.

2003

Jeyaprakash, A. A., Katiyar, S., Swaminathan, C.P., Sekar, K., Surolia, A. & Vijayan, M. (2003). Structural Basis of the Carbohydrate Specificities of Jacalin: An X-ray and Modeling Study. J. Mol. Biol. 332, 217-228.

Ramachandraiah, G., Chandra, N.R., Surolia, A. & Vijayan, M.(2003). Computational analysis of multivalency of Lectins: Structures of garlic lectin-oligosachharide complexes and their aggregates.Glycobiology. 13, 765-75.

Ghosh, A. & Bansal, M. (2003) A glossary of DNA structures from A to Z. Acta Cryst. D59, 620-626.

Bansal, M. (2003) DNA structure: Revisiting the Watson-Crick double helix. Curr. Sci. 85, 1556-1563.

* Kanhere, A. & Bansal, M. (2003). An assessment of three dinucleotide parameters to predict DNA curvature by quantitative comparison to experimental data. Nucl. Acids Res. 31, 2647-2658.

Paul, B.D., Kanhere, A., Chakraborty, A., Bansal, M. & Nagaraja, V. (2003). Identification of the domains for DNA binding and transactivation function of C Protein from bacteriophage Mu. Proteins Str. Fn. Genet. 52, 272-282.

* Madhumalar, A. & Bansal, M. (2003). Structural insights into effect of hydration and ions on A-tract DNA – A molecular Dynamics Study. Biophys. J. 85, 1805-1816.

Mondal, S., Jaishankar, S. P. & 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.

Natesh, R., Manikandan, K., Bhanumoorthy, P., Viswamitra, M. A. & Ramakumar, S. (2003). Thermostable xylanase from Thermoascus aurantiacus at ultrahigh resolution (0.89 A) at 100 K and atomic resolution (1.11 A) at 293 K refined anisotropically to small-molecule accuracy. Acta Cryst. D59, 105-117.

Muralidharan, J., Suguna, K., Surolia, A. & Surolia N. (2003). Exploring the interaction energies for the binding of hydroxydiphenyl ethers to enoyl-acyl carrier protein reductases. J. Biomol. Struct. Dyn. 20, 589-594.

Shanthi, V., Selvarani, P., Kiran Ch. K., Mohire, C. S. & Sekar, K. (2003). SSEP: Secondary Structural Elements of Proteins. Nucl. Acids Res. 31, 3404-3405.

Shanthi, V., Rajesh, C. K., Jayalakshmi, J., Vijay, V. G. & Sekar, K. (2003). WAP: water analysis package - a Web-based package to calculate geometrical parameters between water oxygen and protein atoms. J. Appl. Cryst. 36, 167-168.

Hussain, A. S. Z., Kiran, Ch. K., Rajesh, C. K., Sheik, S. S. & Sekar, K. (2003). SEM: Symmetry Equivalent Molecules - A web based GUI to generate and visualize the Macromolecules. Nucl. Acids Res. 31, 3356-3358.

Sheik, S. S., Sundararajan, P., Shanthi, V. & Sekar, K. (2003). CAP: Conformation Angles Package - Displaying the conformation angles of side chains in proteins. Bioinformatics, 19, 1043-1044.

Sheik, S. S., Ananthalakshmi, P., Ramya, G. B. & Sekar, K. (2003). CADB: Conformational Angles DataBase of proteins. Nucl. Acids Res. 31, 448-451.

Ishu, S., Vijay, V. G., Soma, D., Sekar, K. & Guru, T. N. R. (2003). C-halogen...pi Interactions in Proteins: A Database Study. Cryst. Engg. 6, 69-77.

Gowri, V. S., Pandit, S. B., Karthik, P. S., Srinivasan, N. & Balaji, S. (2003). Integration of related sequences with protein three-dimensional structural families in an updated version of PALI database Nucl. Acids Res. 31, 486-488.

Krupa, A., Sandhya, K., Srinivasan, N. & Jonnalagadda, S. (2003). A conserved domain in the prokaryotic bifunctional FAD synthetases can potentially catalyze nucleotide transfer. Trends Biochem. Sci. 28, 10-13.

Rahaman, A., Srinivasan, N., Shamala, N. & Shaila, M. S. (2003). Fusion Core Complex of Peste des Petits Ruminants Virus is a Six-Helix Bundle Assembly. Biochemistry, 42, 922-931.

Pudi, R., Abhiman, S., Srinivasan, N. & Das, S. (2003). Hepatitis C virus Internal Ribosome Entry Site-mediated translation is stimulated by specific interaction of independent regions of human La autoantigen. J. Biol. Chem. 278, 12231-12240.

Pandit, S. B. & Srinivasan, N. (2003). Survey for G-proteins in the prokaryotic genomes: Prediction of functional roles based on classification. Proteins Str. Fn. Genet. 52, 585-597.

Sopory, S., Balaji, S., Srinivasan, N. & Visweswariah, S. S. (2003). Modeling and mutational analysis of the GAF domain of the cGMP-binding, cGMP-specific phosphodiesterase PDE5. FEBS Lett. 539, 161-166.

Eswar, N., Ramakrishnan, C. & Srinivasan, N. (2003). Stranded in isolation: Structural role of isolated extended-strands in proteins. Protein Eng. 16, 331-339.

Rekha, N. & Srinivasan, N. (2003). Structural basis of regulation and substrate specificity of protein kinase CK2 deduced from the modeling of protein-protein interactions. BMC Struct. Biol. 3, 4.1-4.13

Shenoy, A. R., Srinivasan, N., Subramaniam, M. & Visweswariah, S. S. (2003). Mutational analysis of Mycobacterium tubercolosis Rv1625c adenylyl cyclase: Residues that confer nucleotide specificity contribute to dimerization. FEBS Lett. 545, 253-259.

Balaji, S., Aruna, S. & Srinivasan, N. (2003). Tolerance to the substitution of buried apolar residues by charged residues in the homologous protein structures. Proteins Str. Fn. Genet. 53, 783-791.

* Sandhya, S., Kishore, S., Sowdhamini, R. & Srinivasan, N. (2003). Effective detection of remote homologues by searching in sequence dataset of a protein domain fold. FEBS Lett. 552, 225-230.

Sampath, V., Rekha, N., Srinivasan, N. & Sadhale, P. P. (2003). The conserved and non-conserved regions of Rpb4 are involved in multiple phenotypes in Saccharomyces cerevisiae. J. Biol. Chem. 278, 51566-51576.

Praseeda, M., Pradeep, K. K., Krupa, A., Sri Krishna, S., Leena, S., Rajeev Kumar, R., Cheriyan, J., Mayadevi, M., Srinivasan, N. & Omkumar, R. V. (2003). Influence of a mutation in the ATP-binding region of Calcium/Calmodulin dependent protein kinase II on its interaction with peptide substrates. Biochem. J. 378, 391-397.

Shenoy, A., Sivakumar, K., Krupa, A., Srinivasan, N. & Visweswariah, S. S. (2003). A survey of nucleotide cyclases in Actinobacteria: unique domain organization and expansion of the class III cyclase family in Mycobacterium tuberculosis. Comp. Fnl. Genomics, 5, 17-38.

Badireenath, K. & Chandra, N. R. (2003) Determinants of histamine recognition: Implications for the design of antihistamines. Biochem. Biophys. Res. Commun. 309, 425-431.

Ramachandraiah, G., Chandra, N. R., Surolia, A. & Vijayan, M. (2003). Computational analysis of multivalency in lectins:Structures of garlic-lectin-oligosaccharide complexes and their aggregates. Glycobiology, 13, 765-775.

Bharath, M. M., Chandra, N. R. & Rao, M. R. S. (2003). Molecular modeling of the chromatosome particle. Nucl. Acids Res. 31, 4264-4274.

Prasad, T., Prathima, M. N. & Chandra, N. (2003). Detection of hydrogen-bond signature patterns in protein families. Bioinformatics, 19, 167-168.

Shobini, J., Mishra, A. K. & Chandra, N. (2003). Conformation of gramicidin-A in CTAB micellar media. J. Photochem. Photobiol. B. 70, 117-124.

Datta, S., Ganesh, N., Chandra, N. R., Muniyappa, K. & Vijayan, M. (2003). Structural studies on MtRecA-nucleotide complexes: insights into DNA and nucleotide binding and the structural signature of NTP recognition. Proteins, 50, 474-485.

Bhattacharyya, C., Grate, L. R., Rizki, A., Radisky, D., Molina, F. J., Jordan, M. I., Bissell, M. J. & Mian, I. S. (2003). Simultaneous relevant feature identification and classification in high-dimensional spaces: Application to molecular profiling data. Signal Processing, 83, 729-743.

Srikanta, B., Haritsa, J. & Sen, U. (2003). The Building of BODHI, a Bio-diversity Database System. Information Systems, Elsevier Science Publishers, 28, 347-367.

Truccolo, W., Rangarajan, G., Chen, Y. & Ding, M. (2003). Analyzing stability of equilibrium points in neural networks: A general approach. Neural Net. 16, 1453-1460.

2002

Kirthi, N., Shubha, P. M., Murthy, M. R. N. & H. S. Savithri. (2002). Evidence for recombination among the tomato leaf curl virus strains/species from Bangalore, India. Arch. Virol. 147, 255-272.

Madhusudhan, M. S., Sanjeev, B. S. & Vishveshwara, S. (2002). Computer modeling and molecular dynamics simulations of ligand bound complexes of bovine Angiogenin: Dinucleotide topology at the active-site of Rnase A family proteins. Proteins Str. Fn. Genet. 45, 30-39.

Brinda, K.V., Kannan, N. & Vishveshwara, S. (2002). Analysis of homodimeric protein interfaces by graph spectral methods. Protein Eng. 15, 265-277.

Sanjeev, B.S. & Vishveshwara, S. (2002). Essential dynamics and sidechain hydrogen bond cluster studies in eosinophil cationinc protein. Eur. Phys. J. D, 20, 601-608.

Vishveshwara, S., Brinda, K.V. & Kannan, N. (2002). Protein structure: Insights from graph theory, J. Theor. Comput. Chem. 1, 187-211.

Kant, S., Bagaria, A. & Ramakumar, S. (2002). Putative homeodomain proteins identified in prokaryotes based on pattern and sequence similarity. Biochem. Biophys. Res. Commun. 299, 229-232.

Rudresh, Jain, R., Dani, V., Mitra, A., Srivastava, S., Sarma, S. P., Varadarajan, R. & Ramakumar, S. (2002). Structural consequences of replacement of an alpha-helical Pro residue in Escherichia coli thioredoxin. Protein Eng. 15, 627-633.

Unniraman, S., Prakash, R. & Nagaraja, V. (2002). Conserved economics of transcription terminators in eubacteria. Nucl. Acids Res. 30, 675-684.

Sheik, S. S., Sundararajan, P., Hussain, A. S. Z. & Sekar, K. (2002). Ramachandran plot on the web. Bioinformatics, 18, 1548-1549.

Hussain, A. S. Z., Shanthi, V., Sheik, S. S., Jeyakanthan, J., Selvarani, P. & Sekar, K. (2002). PDB Goodies - a web-based GUI to manipulate the Protein Data Bank file. Acta Cryst. D58, 1385-1386.

* Pandit, S. B., Gosar, D., Abhiman, S., Sujatha, S., Dixit, S. S., Mhatre, N. S., Sowdhamini, R. & Srinivasan, N. (2002). SUPFAM - A database of potential protein superfamily relationships derived by comparing sequence-based and structure-based families: Implications for structural genomics and function annotation in genomes. Nucl. Acids Res. 30, 289-293.

Krupa, A. & Srinivasan, N. (2002). Lipopolysaccharide phosphorylating enzymes encoded in the genomes of Gram-negative bacteria are related to the eukaryotic protein kinases. Prot. Sci. 11, 1580-1584.

Gupta, S., Pandit, S. B., Srinivasan, N. & Chatterji, D. (2002). Proteomics analysis of carbon starved Mycobacterium smegmatis: Induction of Dps like protein. Protein Eng. 15, 503-511.

Shenoy, A. R., Srinivasan, N. & Visweswariah, S. S. (2002). The ascent of nucleotide cyclases: conservation and evolution of a theme. J. Biosci. 27, 85-91.

* Eswar, N., Nagarajaram, H. A., Ramakrishnan, C. & Srinivasan, N. (2002). Influence of solvent molecules on the stereochemical code of glycyl residues in proteins. Proteins Str. Fn. Genet. 49, 326-334.

Sehrawat, S., Srinivasan, N. & Gopinathan, K. P. (2002). Functional characterization and structural modeling of late gene expression factor 4 from Bombyx mori nucleopolyhedrovirus. Biochem. J. 368, 159-169.

Krupa, A. & Srinivasan, N. (2002). Repertoire of protein kinases encoded in the draft version of the human genome: Atypical variations and uncommon domain combinations. Genome Biol. 3, 66.1-66.14.

Bharath, M. M., Chandra, N. R. & Rao, M. R. S. (2002). Prediction of an HMG-box fold in the C-terminal domain of histone H1: insights into its role in DNA condensation. Proteins, 49, 71-81.

Bharath, M. M., Ramesh, S., Chandra, N. R. & Rao, M. R. S. (2002). Identification of a 34 amino acid stretch within the C-terminus of histone H1 as the DNA-condensing domain by site-directed mutagenesis. Biochemistry, 41, 7617-7627.

Pal, D., Suhnel, J. & Weiss, M. S. (2002). New principles of protein structure: nests, eggs--and what next? Angew. Chem. Int. Ed. Engl. 41, 4663-4665.

* Pal, D. & Chakrabarti, P. (2002). On residues in the disallowed region of the Ramachandran map. Biopolymers, 63, 195-206.

* Bhattacharyya, R., Pal, D. & Chakrabarti, P. (2002). Secondary structures at polypeptide-chain termini and their features. Acta Cryst. D58, 1793-1802.

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2007

Ahuja, R., Singhal, N. K., Ramanujam, B., Ravikumar, M. & Rao, C. P. (2007). Experimental and Computational Studies of the Recognition of Amino Acids by Galactosyl-imine and -amine Derivatives: An Attempt to Understand the Lectin-Carbohydrate Interactions. J. Org. Chem. 72, 3430-3442.

Chaudhary, N., Bhartiya, S. & Venkatesh, K. V. (2007). System-level Analysis of Tryptophan Regulation in Escherichia coli – Performance under Starved and Well-fed Conditions. IET Syst. Biol. (In Press).

Gayen, K., Gupta, M. & Venkatesh, K. V. (2007). Elementary mode analysis to study the preculturing effect on the metabolic state of Lactobacillus rhamnosus during growth on mixed substrates. In Silico Biol. 7, 0012.

Gayen, K. & Venkatesh, K. V. (2007). A phenomenological model to represent the kinetics of growth by Corynebacterium glutamicum for lysine production. J. Ind. Microbiol. Biotech (In Press).

Gayen, K. & Venkatesh, K. V. (2007). Quantification of cell size distribution as applied to the growth of Corynebacterium glutamicum. Microbiol. Res. (In Press).

Idicula-Thomas, S. & Balaji, P. V. (2007). Correlation between the structural stability and aggregation propensity of proteins. In Silico Biol. 7, 0023.

Idicula-Thomas, S. & Balaji, P. V. (2007). Protein aggregation: a perspective from amyloid and inclusion body formation. Curr. Sci. 92, 758-767.

Joshi, R. R. (2007). A Decade of Computing to Traverse The Labyrinth of Protein Domains. Curr. Bioinformatics (In Press).

Joshi, R. R. & Samant, V. V. (2007). Bayesian Data Mining of Protein Domains Gives Efficient Predictive Algorithm and New Insight. J. Mol. Mod. 13, 275-282.

Mutalik, V. & Venkatesh, K. V. (2007). A theoretical steady state analysis indicates that induction of Escherichia coli glnALG operon can display all-or-none behavior. BioSystems, (In Press).

Patel, R. Y. & Balaji, P. V. (2007). Characterization of the conformational and orientational dynamics of ganglioside GM1 in a dipalmitoylphosphatidylcholine bilayer by molecular dynamics simulations. Biochim. Biophys. Acta. (Biomembranes). (In Press).

Patel, R. Y. & Balaji, P. V. (2007). Fold recognition and comparative modeling of human beta3GalT I, II, IV, V and VI and beta3GalNAcT I: prediction of residues conferring acceptor substrate specificity. J. Mol. Graph. Model. (In Press).

Patel, S., Balaji, P. V. & Sasidhar, Y. U. (2007). The sequence TGAAKAVALVL from glyceraldehyde-3-phosphate dehydrogenase displays structural ambivalence and interconverts between alpha-helical and beta-hairpin conformations mediated by collapsed conformational states. J. Pept. Sci. 13, 314-326.

Porwal, G., Jain, S., Babu, S. D., Singh, D., Nanavati, H. & Noronha, S. (2007). Protein structure prediction aided by geometrical and probabilistic constraints. J. Comput. Chem. (In Press).

Rana, S., Kundu, B. & Durani, S. (2007). A double catgrip mixed L and D mini-protein only 20 residues long. Bioorg. Med. Chem. 15, 3874-3882.

Rawool, S. & Venkatesh, K. V. (2007). Steady state approach to model gene regulatory networks - Simulation of microarray experiments. BioSystems (In Press).

Sengupta, N., Vinod, P. K. & Venkatesh, K. V. (2007). Crosstalk between cAMP-PKA and MAP kinase pathways is a key regulatory design necessary to regulate FLO11 expression. Biophys. Chem. 125, 59-71.

Sujatha, M. S., Sasidhar, Y. U. & Balaji, P. V. (2007). MP2/6-311++G(d,p) study on galactose-aromatic residue analog complexes in different position-orientations of the saccharide relative to aromatic residues. J. Mol. Struct. (Theochem). (In Press).

* The NMITLI-BioSuite Team. (2007). BioSuite: a comprehensive bioinformatics software package (a unique industry-academia collaboration). Curr. Sci. 92, 29-38.

2006

Bapat, P. M., Bhartiya, S., Venkatesh, K. V. & Wangikar, P. P. (2006). A structured kinetic model to represent the utilization of multiple substrates in complex media during rifamycin B fermentation. Biotech. Bioeng. 93, 779-790.

Bapat, P. M., Das, D., Sohoni, S. V. & Wangikar, P. P. (2006). Hierarchical amino acid utilization and its influence on fermentation dynamics: rifamycin B fermentation in Amycolatopsis mediterranei S699, a case study. Microb. Cell Fact. 5, 32.

Bapat, P. M., Padiyar, N. U., Dave, N. N., Dash, S., Bhartiya, S. & Wangikar, P. P. (2006). Model based optimization of substrate feeding recipe for rifamycin fermentation. AIChE J. 52, 4248-4257.

Bapat, P. M., Sohoni, S. V., Moses, T. A. & Wangikar, P. P. (2006). A cybernetic model to predict the effect of freely available nitrogen substrate on rifamycin B production in complex media. Appl. Microbiol. Biotechnol. 72, 662-670.

Beuria, T. K., Shah, J. H., Santra, M. K., Kumar, V. & Panda, D. (2006). Effects of pH and ionic strength on the assembly and bundling of FtsZ protofilaments: a possible role of electrostatic interactions in the bundling of protofilaments. Int. J. Biol. Macromol. 40, 30-39.

Bhartiya, S., Chaudhary, N., Venkatesh, K. V. & Doyle, III F. J. (2006). Multiple feedback loop design in the tryptophan regulatory network of Escherichia coli suggests a paradigm for robust regulation of processes in series. J. R. Soc. Interface, 3, 383-391.

Chandrasekaran, S., Bhartiya, S. & Wangikar, P. P. (2006). Substrate specificity of lipases in alkoxycarbonylation reaction: QSAR model development and experimental validation. Biotechnol. Bioeng. 94, 554-564.

Gayen, K. & Venkatesh, K. V. (2006). Analysis of optimal phenotypic space using elementary modes as applied to Corynebacterium glutamicum. BMC Bioinformatics, 7, 445.

* Idicula-Thomas, S., Kulkarni, A. J., Kulkarni, B. D., Jayaraman, V. K.& Balaji, P. V. (2006). A support vector machine-based method for predicting the propensity of a protein to be soluble or to form inclusion body on over-expression in Escherichia coli. Bioinformatics, 22, 278-284.

Joshi, R. R. & Gupta, V. K. (2006). Data Mining of VDJ Genes Reveals Interesting Clues. Protein. Pept. Lett. 13, 587-593.

Joshi, R. R. & Samant, V. V. (2006). Fast Prediction of Protein Domain Boundaries using Conserved Local Patterns. J. Mol. Mod. 12, 943-952.

Joshi, S., Rana, S., Wangikar, P. & Durani, S. (2006). Computational design of proteins stereochemically optimized in size, stability, and folding speed. Biopolymers, 83, 122-134.

Mutalik, V. K. & Venkatesh, K. V. (2006). Effect of the MAPK cascade structure, nuclear translocation and regulation of transcription factors on gene expression. BioSystems, 85, 144-157.

Patel, R. Y. & Balaji, P. V. (2006). Identification of linkage-specific sequence motifs in sialyltransferases. Glycobiology, 16, 108-116.

Patel, S., Sista, P., Balaji, P. V. & Sasidhar, Y. U. (2006). Beta-hairpins with native-like and non-native hydrogen bonding patterns could form during the refolding of staphylococcal nuclease. J. Mol. Graph. Model. 25, 103-115.

Ramakrishnan, V., Ranbhor, R., Kumar, A. & Durani, S. (2006). The link between sequence and conformation in protein structures appears to be stereochemically established. J. Phys. Chem. B, 110, 9314-9323.

Ranbhor, R., Ramakrishnan, V., Kumar, A. & Durani, S. (2006). The interplay of sequence and stereochemistry in defining conformation in proteins and polypeptides. Biopolymers, 83, 537-545.

Sujatha, M. S. & Balaji, P. V. (2006). Fold recognition and comparative modeling of human alpha2,3-sialyltransferases reveal their sequence and structural similarities to CstII from Campylobacter jejuni. BMC Struct. Biol. 6, 9.

2005

Bhat, P. J & Venkatesh, K. V. (2005). Stochastic variation in the concentration of a repressor activates GAL genetic switch: Implications in evolution of regulatory network. FEBS Lett. 579, 597-603.

* Gupta, K., Thomas, D., Vidya, S. V., Venkatesh, K. V. & Ramakumar, S. (2005). Detailed protein sequence alignment based on Spectral Similarity Score (SSS). BMC Bioinformatics, 6, 105.

Idicula-Thomas, S. & Balaji, P. V. (2005). Understanding the relationhip between the primary structure of proteins and their amyloidogenic propensity: clues from inclusion body formation. Prot. Eng. Des. Sel. 18, 175-180.

Idicula-Thomas, S. & Balaji, P. V. (2005). Understanding the relationship between the primary structure of proteins and their propensity to be soluble on overexpression in Escherichia coli. Protein Sci. 14, 582-592.

Jyothi, S., Mustafi, S. M., Chary, K. V. R & Joshi, R. R. (2005). Structure Prediction of a Multi-domain EF-hand Ca2+ Binding Protein by PROPAINOR. J. Mol. Mod. 11, 481-488.

Mutalik, V. K. & Venkatesh, K. V. (2005). Quantification of the glycogen cascade system: the ultrasensitive responses of liver glycogen synthase and muscle phosphorylase are due to distinctive regulatory designs. Theor. Biol. Med. Model. 2, 19.

Patel, R. Y. & Balaji, P. V. (2005). Effect of the choice of pressure coupling method on the spontaneous aggregation of DPPC molecules. J. Phys. Chem. B, 109, 14667-14674.

Ramakrishnan, V., Ranbhor R. & Durani, S. (2005). Simulated folding in polypeptides of diversified molecular tacticity: implications for protein folding and de novo design. Biopolymers, 78, 96-105.

Rana, S., Kundu, B. & Durani, S. (2005). A small peptide stereochemically customized as a globular fold with a molecular cleft. Chem. Commun. 2005, 207-209.

Sujatha, M. S., Sasidhar, Y. U. & Balaji, P. V. (2005). Insights into the role of aromatic residue in galactose-binding sites: MP2/6-311G++** study on galactose- and glucose-aromatic residue analog complexes. Biochemistry, 44, 8554-8562.

Tendulkar, A.V., Sohoni, M. A., Ogunnaike, B. & Wangikar, P. P. (2005). A geometric invariant-based framework for the analysis of protein conformational space. Bioinformatics, 21, 3622-3628.

Verma, M., Bhat, P. J. & Venkatesh, K. V. (2005). Steady state analysis of glucose repression reveals hierarchical expression of proteins under Mig1p control in Saccharomyces cerevisiae. Biochem. J. 388, 843-849.

2004

Giri, L., Mutalik, V. K. & Venkatesh, K. V. (2004). A steady state analysis indicates that negative feedback regulation of PTP1B by Akt elicits bistability in insulin-stimulated GLUT4 translocation. Theor. Biol. Med. Model. 1, 2.

Mutalik, V. K., Singh, A. P., Edwards, J. S. & Venkatesh, K. V. (2004). Equilibrium analysis of allosteric interactions shows zero order effects. Cell Biochem. Biophy. 41, 179-192.

Mutalik, V. K., Singh, A. P., Edwards, J. S. & Venkatesh, K. V. (2004). Robust global sensitivity in multiple enzyme cascade system explains how the downstream cascade structure may remain unaffected by cross-talk. FEBS Lett. 558, 79-84.

Mutalik, V. K. & Venkatesh, K. V. (2004). Steady State Analysis of Signaling Pathways in Living Systems: Use of Dimensionless Parameters Akin to Chemical Plants. Ind. Chem. Eng. B, 46, 261-265.

Patel, S., Venkatesh, K. V. & Edwards, J. S. (2004). An integrated mechanistic model for transcription-coupled nucleotide excision repair. DNA Repair, 3, 343-348.

Poolman, M. G., Venkatesh, K. V., Pidcock, M. K. & Fell, D. A. (2004). A Method for the Determination of Flux in Elementary Modes, and its Application to Lactobacillus rhamnosus. Biotech. Bioeng. 88, 601-612.

Ramakrishnan, V., Ranbhor, R. & Durani, S. (2004). Existence of specific "folds" in polyproline II ensembles of an "unfolded"alanine peptide detected by molecular dynamics. J. Am. Chem. Soc. 126, 16332-16333.

Rana, S., Kundu, B. & Durani, S. (2004). Stereospecific peptide folds. A rationally designed molecular bracelet. Chem. Commun. 2004, 2462-2463.

Ruhela, A., Verma, M., Edwards, J. S., Bhat, P. J., Bhartiya, S. & Venkatesh, K. V. (2004). Autoregulation of Regulatory Proteins is Key for Dynamic Operation of GAL Switch in Saccharomyces cerevisiae. FEBS Lett. 576, 119-126.

Sujatha, M. S. & Balaji, P. V. (2004). Identification of common structural features of binding sites in galactose-specific proteins. Proteins, 55, 44-65.

Sujatha, M. S., Sasidhar, Y. U. & Balaji, P. V. (2004). Energetics of galactose- and glucose-aromatic amino acid interactions: implications for binding in galactose-specific proteins. Prot. Sci. 13, 2502-2514.

Tendulkar, A. V., Joshi, A. A., Sohoni, M. A. & Wangikar, P. P. (2004). Clustering of Protein Structural Fragments Reveals Modular Building Block Approach of Nature. J. Mol. Biol. 338, 611-629.

Venkatesh, K. V., Bhartiya, S. & Ruhela, A. (2004). Multiple feedback loops are key to a robust dynamic performance of tryptophan regulation in Escherichia coli. FEBS Lett. 563, 234-240.

Verma, M., Bhat, P. J., Bhartiya, S. & Venkatesh, K. V. (2004). A Steady State Modeling Approach to Validate in vivo Mechanism of GAL Regulatory Network in Saccahromyces cerevisiae. Eur. J. Biochem. 271, 4064-4074.

Verma, M., Bhat, P. J. &Venkatesh, K. V. (2004). Expression of GAL genes in a mutant strain of Saccharomyces cerevisiae lacking GAL80: Quantitative Model and Experimental Verification. Biotechnol. Appl. Biochem. 39, 89-97.

2003

Bhartiya, S., Rawool, S. & Venkatesh, K. V. (2003). Dynamic Model of Escherichia coli Tryptophan Operon Shows an Optimal Structural Design. Eur. J. Biochem. 270, 2644-2651.

Joshi, R. R. & Jyothi, S. (2003). Ab-initio Prediction and Reliability of Protein Structural Genomics by PROPAINOR. Comput. Biol. Chem. 27, 241-252.

Jyothi, S. & Joshi, R. R. (2003). Ab-initio Computation of the 3d-Structure of Proteins by Nonparametric Statistical Methods – Medium and Short Range Distance Estimates. Sankhya, 65, 593-611.

Jyoti, B. D., Suresh, A. K. & Venkatesh, K. V. (2003). An optimal model to represent the kinetics of growth and product formation by Lactobacillus rhamnosus on multiple substrates. J. Biosci. Bioeng. 96, 481-486.

Mohanraja, K., Dhanasekaran, M., Kundu, B. & Durani, S. (2003). Mechanism-based protein design: attempted "nucleation-condensation" approach to a possible minimal helix-bundle protein. Biopolymers, 70, 355-363.

Mutalik, V. K., Shah, P. & Venkatesh, K. V. (2003). Allosteric Interactions and Bifunctionality Make the Response of Glutamine Synthetase Cascade System of Escherichia coli Robust and Ultrasensitive. J. Biol. Chem. 278, 26327-26332.

Santra, M. K. & Panda, D. (2003). Detection of an intermediate during unfolding of bacterial cell division protein FtsZ: loss of functional properties precedes the global unfolding of FtsZ. J. Biol. Chem. 278, 21336-21343.

Sureshkumar, S. V., Phale, P. S., Durani, S. & Wangikar, P. P. (2003). Combined sequence and structure analysis of the fungal laccase family. Biotechnol. Bioeng. 83, 386-394.

Tendulkar, A V., Wangikar, P. P., Sohoni, M. A., Samant, V. V. & Mone, C. Y. (2003). Parameterization and Classification of Protein Universe via Geometric Techniques. J. Mol. Biol. 334, 157-172.

Verma, M., Bhat, P. V. & Venkatesh, K. V. (2003). Quantitative analysis of GAL genetic switch of Saccharomyces cerevisiae reveals that nucleocytoplasmic shuttling of Gal80p results in a highly sensitive response to galactose. J. Biol. Chem. 278, 48764-48769.

Wangikar, P. P., Tendulkar, A. V., Ramya, S., Mali, D. & Sarawagi, S. (2003). Functional Sites in Protein Families uncovered via an Automated and Objective Graph Theoretic Approach. J. Mol. Biol. 326, 955-978.

2002

Joshi, R. R. & Bhuvaneswaran, N. (2002). Prediction and Analysis of Vaccination Possibilities in Autoimmune Diseases – An Application of Artificial Immune System. J. Biol. Syst. 10, 107-126.

Joshi, R. R. & Jyothi, S. (2002). Ab-initio Structure of Human Seminal Plasma Prostatic Inhibin Gives Significant Insight into its Biological Functions. J. Mol. Model. 8, 50-57.

Vasudevan, S. V. & Balaji, P. V. (2002). Comparative analysis of ganglioside conformations by MD simulations: implications for specific recognition by proteins. J. Mol. Struct. (Theochem). 583, 215-232.

Vasudevan, S. V. & Balaji, P. V. (2002). Conformation, orientation and dynamics of dodecylphosphocholine in micellar aggregate: a 3.2 ns molecular dynamics simulation study. Ind. J. Biochem. Biophys. 39, 87-92.

Vasudevan, S. V. & Balaji, P. V. (2002). Molecular dynamics simulation of alpha2-8-linked disialoside: conformational flexibility and implications for binding to proteins. Biopolymers, 63, 168-180.

INDIAN INSTITUTE OF TECHNOLOGY, MADRAS.

2007

Gangadhar, G., Joseph, D. & Chakravarthy, V. S. (2007). An oscillatory neuromotor model of handwriting generation, International Journal of Document Analysis and Recognition (in press).

INDIAN INSTITUTE OF TECHNOLOGY, New Delhi.

2007

Jain, T. and Jayaram, B. (2007). A computational protocol for predicting the binding affinities of zinc containing metalloprotein-ligand complexes. Proteins, 67, 1167-1178.

Shaikh, S. A. & Jayaram, B. (2007). A Swift All-Atom Energy Based Computational Protocol to Predict DNA ligand Binding Affinity and Tm. J. Med. Chem. (In Press).

Shaikh, S. A., Jain, T., Sandhu, G., Latha, N. and Jayaram, B. (2007). From Drug Target to Leads-Sketching, A Physicochemical Pathway for Lead Molecule Design In Silico. Curr. Pharma. Desig. (In Press).

Thukral, L., Shenoy, S. R., Bhushan, K. & Jayaram, B. (2007) ProRegIn: A regularity index for the selection of native-like tertiary structures of proteins. J. Biosci. 32, 71-81.

Bajaj, K. & Bhaumik, B. (2007). Adaptation-induced suppression and facilitation: Effect of intra- and extracellular ionic disturbances. Neurocomputing, 10, 1695-1701.

Bajaj, K & Bhaumik, B. (2007). Attentional modulation of tilt aftereffect caused by cholinergic basal forebrain projections. Neural Inf. Proc. Lett. Rev. (In press).

2006

Jayaram, B., Bhushan, K., Shenoy, S. R., Narang, P., Bose, S., Agrawal, P., Sahu, D. & Pandey, V.S. (2006). Bhageerath : An Energy Based Web Enabled Computer Software Suite for Limiting the Search Space of Tertiary Structures of Small Globular Proteins. Nucl. Acids Res. 34, 6195-6204.

Dutta, S., Singhal, P., Agrawal, P., Tomer, R., Kritee, Khurana, E. & Jayaram, B. (2006). A Physico-Chemical Model for Analyzing DNA sequences. J. Chem. Inf. Model. 46, 78-85.

Narang, P., Bhushan, K., Bose, S., and Jayaram, B. (2006). Protein structure evaluation using all-atom energy based empirical scoring function. J. Biomol. Struct. Dyn. 23, 385-406.

Jayaram, B., Latha, N., Jain, T., Sharma, P., Gandhimathi, A & Pandey, V.S. (2006). Sanjeevini: A Comprehensive Active-Site Directed Lead Design Software. Ind. J. Chem. 45A, 21-33.

* Garg, A. R. & Bhaumik, B. (2006). Ratio of Average Inhibitory to Excitatory Conductance Modulates the Response of Simple Cell. Lect. Note. Comp. Sci. 4232, 82-89.

2005

Jain, T & Jayaram, B. (2005). An all atom energy based computational protocol for predicting binding affinities of protein-ligand complexes. FEBS Lett. 579, 6659-6666.

Narang, P., Bhushan, K., Bose, S. & Jayaram, B. (2005). A computational pathway for bracketing native-like structures for small alpha helical globular proteins. Phys. Chem. Chem. Phys. 7, 2364-2375.

Latha, N & Jayaram, B. (2005). A Binding Affinity Based Computational Pathway for Active-Site Directed Lead Molecule Design: Some Promises and Perspectives. Drug Des. Rev. Online. 2, 145-165.

* Garg, A. R., Bhaumik, B. & Obermayer, K. (2005). Variable Discharge Pattern and Contrast Invariant Orientation Tuning of a Simple Cell: A Modelling Study. Neural Inf. Proc. Lett. Rev. 6, 59-68.

Mathur, M. & Bhaumik, B. (2005). Study of Sptail Frequency Selectivity and its Spatial Organization in the Visual Cortex through a Feedforward Model. Neurocomputing, 65, 85-91.

Bhaumik, B., Agarwal, A. & Manohar, M. (2003). Receptive Field Properties of Near Neighbour Orientation Selective Neurons in the Visual Cortex: A Modelling Study. Int. J. Neural Syst. 15, 31-40.

* Garg, A. R., Obermayer, K. & Bhaumik, B. (2005). Development of feed-forward Receptive Field Structure of a Simple Cell and its Contribution to the Orientation Selectivity: A Modelling Study. Int. J. Neural Syst. 15, 55-70.

2004

Jayaram, B. & Jain, T. (2004). The role of water in protein-DNA recognition. Annu. Rev. Biophys. Biomol. Struct. 33, 343-361.

Shaikh, S.A., Ahmed, S.R. & Jayaram, B. (2004). A molecular thermodynamic view of DNA-drug interaction: A case study of 25 minor groove binders. Arch. Biochem. Biophys. 429, 81-99.

Latha, N., Jain, T., Sharma, P. & Jayaram, B. (2004). A free energy based computational pathway from chemical templates to lead compounds: a case study of COX-2 inhibitors. J. Biomol. Struct. Dyn. 21, 791-804.

Bhaumik, B., Agarwak, A., Mathur, M. & Manohar, M. (2004). A Model That Captures Receptive Field Properties of Orientation Selective Neurons in the Visual Cortex. Lect. Note. Comput. Sci. 3316, 57-63.

Mathur, M. & Bhaumik, B. (2004). Orientation Map Emerges in Parallel with the Formation of Receptive Fields in a Feedforward Neurotrophic Model. Lect. Note. Comput. Sci. 3316, 84-89.

2003

Bhaumik, B. & Mathur, M. (2003). Receptive Fields and Orientation Selectivity of Simple Cells in Visual Cortex, IETE J. Res. 49, 87-96.

Bhaumik, B. & Mathur, M. (2003). A Cooperation and Competition Based Simple Cell Receptive Field Model and Study of Feed-Forward Linear and Nonlinear Contributions to Orientation Selectivity, J. Comp. Neurosci. 14, 211-227.

2002

Jayaram, B., McConnell, K., Dixit, S.B., Das, A. & Beveridge, D.L. (2002). Free energy component analysis of 40 protein-DNA complexes: A consensus view on the thermodynamics of binding at the molecular level. J. Comput. Chem. 23, 1-14.

* Bhaumik, B. & Garg, A. R. (2002). Direction-selective simple cells in cat striate cortex: a developmental mode. Neural Net.1, 778 –783.

INDIAN INSTITUTE OF TECHNOLOGY, KANPUR.

Baskaran, A., Sunil, K. V. & Balaji, P. (2006). Circularly Permuted GTP Binding Proteins Need Additional domains for GTP hydrolysis. Nucl. Acids Res. 34, 2196-2205.

Rajeev, M., Sudheer, K. G., Shambhavi, M. & Balaji, P. (2005). Analysis of GTPases carrying hydrophobic amino acid substitutions in lieu of the catalytic glutamine: Implications for GTP hydrolysis. Proteins: Struct. Func. Bioinfo. 59, 332-338.

INDIAN INSTITUTE OF TECHNOLOGY,KHARAGPUR.

2006

Das, D., Badri, P. K., Kumar, N. & Bhattacharya, P. (2006). Simulation and modeling of continuous H_2 production process by Enterobacter cloacae IIT-BT 08 using different bioreactor configuration. Enzyme. Microb. Technol. 31, 867-875.

Chanda, J. & Bandyopadhyay, S. (2006). Molecular dynamics study of surfactant monolayers adsorbed at the oil/water and air/water interfaces. J. Phys. Chem. 110, 23482 –23488.

Srivastava, R., Das, D. R., Wiker, H. G. & Das A. K. (2006). Functional insights from the molecular modeling of a novel two-component system. Biochem. Biophys. Res. Commun. 344, 1327–1333.

Mahendran, B., Ghosh, S. K. & Kundu, S. C. (2006). Molecular phylogeny of silk producing insects (Saturniidae family, Genus, Antheraea) based on 16S ribosomal RNA and cytochrome oxidase genes. J. Genet. 85, 31-38.

Saha, M. & Kundu, S. C. (2006). Molecular identification of tropical tasar silkworm (Antheraea mylitta) ecoraces with RAPD and SCAR markers. Biochem. Genet. 44, 75-88.

Mahendran, B., Acharya, C., Dash, R., Ghosh, S. K. & Kundu, S. C. (2006). Repetitive DNA in tropical tasar silk worm Antheraea mylitta. Gene, 370, 51-57.

Mahendran, B., Padhi, B. K., Ghosh, S. K. & Kundu, S. C. (2006). Genetic variation in ecoraces of tropical tasar silkworm, Antheraea mylitta using RFLP technique. Curr. Sci. 90, 100-103.

Chanda, J. & Bandyopadhyay, S. (2006). Hydrogen bond lifetime dynamics at the interface of a surfactant monolayer. J. Phys. Chem. B, 23, 23443-23444.

Bandyopadhyay, S., Chakraborty, S. & Bagchi, B. (2006). Exploration of the secondary structure specific differential solvation dynamics between the native and molten globule states of the protein HP-36, J. Phys. Chem. B, 110, 20629-20634.

Chanda, J., Chakraborty, S. & Bandyopadhyay, S. (2006). Sensitivity of hydrogen bond lifetime dynamics to the presence of ethanol at the interface of a phospholipid bilayer. J. Phys. Chem. B, 110, 3791-3797.

Bandyopadhyay, S., Chakraborty, S. & Bagchi, B. (2006). Coupling between hydration layer dynamics and unfolding kinetics of HP-36. J. Chem. Phys. 125, 084912.

De, S., Pal, D. & Ghosh, S. K. (2006). Entamoeba histolytica: Computational identification of putative microRNA candidates. Exp. Parasitol. 113, 239-243.

2005

Ghosh, A. K., Datta, A., Mahendran, B. & Kundu, S. C. (2005). Molecular characterization of a Pao-like long terminal repeat retrotransposon, Tamy in saturniid silkworm Antheraea mylitta. Curr. Sci. 89, 539-543.

Mitra, D., Saha, B., Das, D., Wiker, H. G. & Das, A. K. (2005). Correlating sequential homology of Mce1A, Mce2A, Mce3A and Mce4A with their possible functions in mammalian cell entry of Mycobacterium tuberculosis performing homology modeling. Tuberculosis (Edinb). 85, 337-345.

Sen, R. & Babu, S. (2005). Modeling and optimization of the process conditions for biomass production and sporulation of a probiotic culture. Process Biochem. 40, 2531–2538.
Bandyopadhyay, S., Chakraborty, S. & Bagchi, B. (2005). Secondary structure sensitivity of hydrogen bond lifetime dynamics in the protein hydration layer. J. Am. Chem. Soc. 127, 16660-16667.

2004

Sen, R. & Swaminathan, T. (2004). Response surface modeling and optimization to elucidate the effects of inoculum age and size on Surfactin production. Biochem. Eng. J. 21, 141–148.

2003

Nath, K. & Das, D. (2003). Energy and economic analysis of a fermentative hydrogen production process. Bioenergy News, 7, 15-19.

Mishra, S., Mazumdar, P. A., Dey, J. & Das, A. K. (2003). Molecular modeling of RecX reveals its mode of interaction with RecA. Biochem. Biophys. Res. Commun. 312, 615-622.

Das, A. K., Mitra, D., Harboe, M., Nandi, B., Harkness, R. E., Das, D. & Wiker, H. G. (2003). Predicted molecular structure of the mammalian cell entry protein Mce1A of Mycobacterium tuberculosis. Biochem. Biophys. Res . Commun. 302, 442-447.

Pal, M. & Dasgupta, S. (2003). The nature of the turn in omega loops of proteins, Proteins, 51, 591-606.

2002

Modak, J. M., Bandopadhyay, K., Das, D. & Maiti, B. R. (2002). Mathematical model for evaluation of mass transfer limitations in phenol biodegradation by immobilized *Pseudomonas putida*. J. Biotechnol. 87, 211-223.

INDIAN STATISTICAL INSTITUTE, KOLKATA.

2007

Bandyopadhyay, S., Maulik, U. & Roy, D. (2007). Gene Identification: Classical and Computational Intelligence Approaches. IEEE Trans. Syst. Man Cybern. Part C (In press).

Banerjee, M., Mitra, S. & Banka, H. (2007). Evolutionary-Rough feature selection in gene expression data. IEEE Trans. Syst. Man Cybern. Part C: Appl. Rev. (In press).

Nayak, L. & De, R.K. (2007). An algorithm for modularization of MAPK and Calcium signaling pathways: Comparative analysis among different species. J. Biomed. Inform. (In press)

Ray, S. S., Bandyopadhyay, S. & Pal, S. K. (2007). Dynamic Range Based Distance Measure for Microarray Expressions and A Fast Gene Ordering Algorithm. IEEE Trans. Syst. Man Cybern. Part B (In press).

2006

Chaudhuri, P. & Dasgupta, A. (2006). Stationarity and mixing properties of replicating character strings. Statist. Sinica, 16, 29-43.

Mitra, S. & Banka, H. (2006). Multi-objective evolutionary biclustering of gene expression data. Patt. Recognit. 39, 2464-2477.

Mitra, S. & Hayashi, Y. (2006). Bioinformatics with soft computing. IEEE Trans. Syst. Man Cyber. Part C: Appl. Rev. 36, 616-635.

Banka, H. & Mitra, S. (2006). Evolutionary biclustering of gene expressions. ACM Ubiquity, 7, 17-26.

2005

Bandyopadhyay, S. (2005). An Efficient Technique for Superfamily Classification of Amino Acid Sequences: Feature Extraction, Fuzzy Clustering and Prototype Selection. Fuzzy Sets Syst. 152, 5-16.

Bandyopadhyay, S., Bagchi, A. & Maulik, U. (2005). Active Site Driven Ligand Design: An Evolutionary Approach. J. Bioinform. Comput. Biol. 3, 1053-1070.

Basu, A., Chaudhuri, P. & Majumder Partha P. (2005). Identification of polymorphic motifs using probabilistic search algorithms. Genome Res. 15, 67-77.

Mitra, S. (2005). Computational intelligence in Bioinformatics. LNCS Trans. Rough Sets III, LNCS 3400, 134-152.

Ray, S. S., Bandyopadhyay, S., Mitra, P. & Pal, S.K. (2005). Bioinformatics in Neurocomputing Framework. Proc. IEE Circ. Dev. Syst. 152, 556-564.

Chaudhuri, P. & Dasgupta, A. (2005). On some stochastic models for replication of character strings. Stat. Prob. Lett. 75, 230-236.

2003

Basu, A. & Majumder, Partha P. (2003). A comparison of two popular statistical methods for estimating the time to most recent common ancestor (TMRCA) from a sample of DNA sequences. J. Genet. 82, 7-12

Basu, S., Burma, D. P. & Chaudhuri, P. (2003). Words in DNA sequences: some case studies based on their frequency statistics. J. Math. Biol. 46, 479-503.

2002

Chaudhuri, P. & Das, S. (2002). SWORDS: a statistical tool for analysing large DNA sequences. J Biosci. 27, 1-6.

INSTITUTE OF MICROBIAL TECHNOLOGY, CHANDIGARH.

2007

Saha, S., Zack, J., Singh, B. & Raghava, G. P. S. (2007). VGIchan: Prediction and classification of voltage-gated ion channels. Genomics Proteomics & Bioinformatics, 4, 253-258.

* Greenbaum et al. (2007). Towards a consensus on datasets and evaluation metrics for developing B cell epitope prediction tools. J. Mol. Recognit. 20, 75-82.

2006

Kaundal, R., Kapoor, A. S. & Raghava, G. P. S. (2006). Machine learning techniques in disease forecasting: a case study on rice blast prediction. BMC Bioinformatics, 7, 485.

Saha, S. & Raghava, G. P. S. (2006). Prediction of continuous B-cell epitopes in an antigen using recurrent neural network. Protein Struct. Fn. Bioinf. 65, 40-48.

Raghava, G. P. S. & Barton, G. J. (2006). Quantification of the variation in percentage identity for protein sequence alignments. BMC Bioinformatics, 7, 415

Saha, S. & Raghava, G. P. S. (2006). AlgPred: Prediction of allergenic proteins and mapping of IgE epitopes. Nucl. Acids Res. 34, W202-W209.

Kim, J.K., Raghava, G. P. S., Bang, S. & Choi, S. (2006). Prediction of subcellular localization of proteins using pairwise sequence alignment and support vector machine. Patt. Recognit. Lett. 27, 996-1001.

Bhasin, M. & Raghava, G. P. S. (2006). A hybrid approach for predicting promiscuous MHC class I restricted T cell epitopes. J. Biosci. 31, 31–42.

Saha, S. & Raghava, G. P. S. (2006). VICMpred: SVM-based method for the prediction of functional proteins of gram-negative bacteria using amino acid patterns and composition. Genomics Proteomics Bioinformatics, 4, 42-47.

Kumar, M., Verma, R. & Raghava, G. P. S. (2006). Prediction of mitochondrial proteins using support vector machine and hidden markov model. J. Biol. Chem. 281, 5357 - 5363.

Kaur, H. & Raghava, G.P.S. (2006). Prediction of Cα-H...O and Cα-H...π interactions in proteins using recurrent neural network. In Silico Biol. 6, 11.

Singh, M.K., Srivastava, S., Raghava, G. P. S. & Varshney, G.C. (2006). HaptenDB: A comprehensive database of haptens, carrier proteins and anti-hapten antibodies. Bioinformatics, 22, 253-255.

2005

Saha, S., Bhasin, M. & Raghava, G. P. S. (2005). BCIPEP: A database of B-cell epitopes. BMC Genomics, 6, 79.

Garg, A., Kaur, H. & Raghava, G. P. S. (2005). Real value prediction of Solvent accessibility in proteins using multiple sequence alignment and secondary structure. Proteins Str. Fn. Bioinf. 61, 318-324.

The Indian Genome Variation Consortium. (2005). The Indian Genome Variation database (IGVdb): a project overview. Hum. Genet. 118, 1-11.

Bhasin, M. & Raghava, G. P. S. (2005). Pcleavage: A SVM based Method for Prediction of Consitutive and Immuno proteasome Cleavage Sites in Antigenic Sequences . Nucl. Acids Res. 33, W202-W207.

Kumar, M., Bhasin, M., Natt, N.K. & Raghava, G. P. S. (2005). BhairPred: A webserver for Prediction of Beta-hairpins in proteins from Multiple Alignment Information Using ANN and SVM Techniques. Nucl. Acids Res. 33, W154-W159.

Bhasin, M., Garg, A., & Raghava, G. P. S. (2005). PSLpred: prediction of subcellular localization of bacterial proteins. Bioinformatics, 21, 2522-2524.

Raghava, G. P. S. & Han, J. H. (2005) Correlation and prediction of gene expression level from amino acid and dipeptide composition of its protein. BMC Bioinformatics, 6, 59.

Garg, A., Bhasin, M. & Raghava, G. P. S. (2005). SVM-based method for subcellular localization of human proteins using amino acid compositions, their order and similarity search. J. Biol. Chem. 280, 14427-14432.

Bhasin, M. & Raghava, G. P. S. (2005). MHCBN: A comprehensive database of MHC/TAP binders/non-binders and T-cell epitopes. Nucl. Acids Res. 19, 665-666.

Bhasin, M. & Raghava, G. P. S. (2005). GPCRsclass : A web tool for classification of amine type of G-protein coupled Receptors. Nucl. Acids Res. 33, W143-W147.

2004

Bhasin, M. & Raghava, G. P. S. (2004). Prediction of CTL epitopes using QM, SVM and ANN techniques. Vaccine, 22, 3195-3204.

Kaur, H. & Raghava, G. P. S. (2004). A neural network method for prediction of beta-turn types in proteins using evolutionary information. Bioinformatics, 20, 2751-2758.

Kaur, H. & Raghava, G. P. S. (2004). Prediction of Alpha-turns in proteins using PSI-BLAST profiles and secondary structure information. Proteins Str. Fn. Genet. 55, 83-90.

Bhasin, M. & Raghava, G. P. S. (2004). SVM based method for predicting HLA-DRB1*0401 binding peptides in an antigen sequence. Bioinformatics, 12, 421-423.

Bhasin, M. & Raghava, G. P. S. (2004). Analysis and Prediction of affinity of TAP binding peptides using Cascade SVM. Protein Sci. 13, 596-607.

* Sharma, D., Issac, B., Raghava, G. P. S. & Ramaswamy, R. (2004). Spectral Repeat Finder (SRF): Identification of repetitive sequences using fourier transformation. Bioinformatics, 20, 1405-1412.

Natt, N. K., Kaur, H. & Raghava, G. P. S. (2004). Prediction of Transmembrane regions of beta-barrel proteins using ANN and SVM based method. Proteins Str. Fn. Bioinf. 56, 11-18.

Bhasin, M. & Raghava, G. P. S. (2004). ESLpred: SVM Based Method for Subcellular Localization of Eukaryotic Proteins using Dipeptide Composition and PSI-BLAST. Nucl. Acids Res. 32, W414-W419.

Kaur, H. & Raghava, G. P. S. (2004). Role of evolutionary information in prediction of aromatic-backbone NH interactions in proteins. FEBS Lett. 564, 47-57.

Bhasin, M. & Raghava, G. P. S. (2004) Classification of nuclear receptors based on amino acid composition and dipeptide composition. J. Biol. Chem. 279, 23262-23266.

Bhasin, M. & Raghava, G. P. S. (2004). GPCRpred: An SVM Based Method for Prediction of families and subfamilies of G-protein coupled receptors. Nucl. Acids Res. 32, W383-W389.

Issac, B. & Raghava, G. P. S. (2004). EGPred: Prediction of Eukaryotic genes using ab initio methods after combining with sequence similarity approaches. Genome Res. 14, 1756-1766.

Singh, B. (2004) PepBuild: A web server for building structure data of peptides / proteins. Nucl. Acids Res. 32, 559-561.

Luthra-Guptasarma, M. & Singh, B. (2004). HLA-B27 lacking associated beta2-microglobulin rearranges to auto-display or cross-display residues 169-181: A novel molecular mechanism for spondyloarthropathies. FEBS Lett. 575, 1-8.

2003

Kaur, H. & Raghava, G. P. S. (2003) Prediction of Beta-turns in proteins from multiple alignment using neural network. Protein Sci. 12, 627-634.

Bhasin, M., Singh, H. & Raghava, G. P. S. (2003). MHCBN: A comprehensive database of MHC binding and non-binding peptides. Bioinformatics, 19, 665-666.

Singh, H. & Raghava, G. P. S. (2003). ProPred1: Prediction of promiscuous MHC class-I binding sites. Bioinformatics, 19, 1009-1014.

Kaur, H. & Raghava, G. P. S. (2003). A neural network based method for prediction of gama-turns in proteins from multiple sequence alignment. Protein Sci. 12, 923-929.

Kaur, H. & Raghava, G. P. S. (2003). BTEVAL: A server for evaluation of beta-turn prediction methods. J. Bioinform. Comput. Biol. 1, 495-504

Sarin,J., Raghava, G. P. S. & Chakraborti, P. K. (2003). Intrinsic contributions of polar amino acid residues towards thermal stability of an ABC-ATPase of mesophilic origin. Protein Sci. 12, 2118-2120.

Bhasin, M., & Raghava, G. P. S. (2003). Prediction of promiscuous and high affinity mutated MHC binders. Hybrid Hybridomics, 22, 229-234.

Raghava, G. P. S., Searle, S.M., Audley, P.C., Barber J.D. & Barton G.J. (2003). OXBench: Evaluation of protein multiple sequence alignment. BMC Bioinformatics, 4, 47.

2002

Issac, B., Singh H., Kaur, H. & Raghava, G. P. S. (2002). Locating probable genes using fourier transform. Bioinformatics, 18, 196-197

Kaur, H. & Raghava, G. P. S. (2002). BetaTPred: Prediction of Beta-turns in a protein using statistical algorithms. Bioinformatics, 18, 498-499.

Issac, B. & Raghava, G. P. S. (2002). GWFASTA: A server for FASTA search in Eukaryotic and Microbial genomes. Biotechniques, 33, 548-556.

Kaur, H. & Raghava, G. P. S. (2002). An Evaluation of Beta-Turn Prediction Methods. Bioinformatics, 18, 1508-1514.

Singh, H. & Raghava, G. P. S. (2002). Detection of Orientation of MHC Class II Binding Peptides Using Bioinformatics Tools. Biotech Soft. Internet Rep. 3, 146-150.

INSTITUTE OF BIOINFORMATICS AND APPLIED BIOTECHNOLOGY, BANGALORE.

2006

Rathinavelan, T & Yathindra, N. (2006). Base triplet non-isomorphism strongly influences DNA triplex conformation: Effect of non-isomorphic G*GC and A*AT triplets and bending of DNA triplexes. Biopolymers, 82, 443-461.

2005

Sandhu K.S. & Acharya, K.K. (2005). ExPrimer: To design primers from exon-exon junctions. Bioinformatics, 21, 2091-2092.

* Rekha, N., Machado, S. M., Narayanan, C., Krupa, A. & Srinivasan, N. (2005). Interaction interfaces of protein domains are not topologically equivalent across families within superfamilies: Implications for metabolic and signaling pathways. Proteins, 58, 339-353.

Rathinavelan, T. & Yathindra, N. (2005). Molecular dynamics structures of peptide nucleic acid, DNA hybrid in the wild-type and mutated alleles of Ki-ras proto-oncogene. FEBS J. 272, 4055-4070.

2004

* Kanhere, A. & Bansal, M. (2004). DNA Bending and Curvature: A Turning Point in DNA Function, Proc. Indian Natl. Acad. Sci. B70, 239-254.

2003

* Madhumalar, A. & Bansal, M. (2003). Structural insights into the Effect of Hydration and Ions on A-Tract DNA: A Molecular Dynamics Study. Biophy. J. 85, 1805-1816.

* Kanhere, A. & Bansal, M. (2003). An assessment of three dinucleotide parameters to predict DNA curvature by quantitative comparison to experimental data. Nucl. Acids Res. 31, 2647-2658.

INSTITUTE OF GENOMICS AND INTEGRATIVE BIOLOGY, NEW DELHI.

2007

Ganapathi, M., Singh, G. P., Sandhu, K. S., Brahmachari, S. K. & Brahmachari, V. (2007). A whole genome analysis of 5' regulatory regions of human genes for putative cis-acting modulators of nucleosome positioning. Gene, 391, 242-251.

Gupta, S., Bisht, S. S., Kukreti, R., Jain, S. & Brahmachari, S. K. (2007). Boolean network analysis of a neurotransmitter signaling pathway. J. Theor. Biol. 244, 463-469.

2006

Harish, N., Gupta, R., Agarwal, P., Scaria, V. & Pillai, B. (2006). DyNAVacS: an integrative tool for optimized DNA vaccine design. Nucl. Acids Res. 34, W264-W266.

Rawal, P., Kummarasetti, V. B., Ravindran, J., Kumar, N., Halder, K., Sharma, R., Mukerji, M., Das, S. K. & Chowdhury, S. (2006). Genome-wide prediction of G4 DNA as regulatory motifs: role in Escherichia coli global regulation. Genome Res. 16, 644-655.

Sandhu, K. S. & Dash, D. (2006). Conformational flexibility may explain multiple cellular roles of PEST motifs. Proteins. 63, 727-732.

Scaria, V., Hariharan, M., Arora, A. & Maiti, S. (2006). Quadfinder: server for identification and analysis of quadruplex-forming motifs in nucleotide sequences. Nucl. Acids Res. 34, W683-W685.

Sharma, V. K., Sharma, A., Kumar, N., Khandelwal, M., Mandapati, K. K., Horn-Saban, S., Strichman-Almashanu, L., Lancet, D., Brahmachari, S. K. & Ramachandran, S. (2006). Expoldb: expression linked polymorphism database with inbuilt tools for analysis of expression and simple repeats. BMC Genomics, 7, 258.

Singh, G. P., Ganapathi, M., Sandhu, K. S. & Dash, D. (2006). Intrinsic unstructuredness and abundance of PEST motifs in eukaryotic proteomes. Proteins, 62, 309-315.

2005

Chavali, S., Mahajan, A., Tabassum, R., Maiti, S. & Bharadwaj, D. (2005). Oligonucleotide properties determination and primer designing: a critical examination of predictions. Bioinformatics, 21, 3918-3925.

Ganapathi, M., Srivastava, P., Das Sutar, S. K., Kumar, K., Dasgupta, D., Pal, S. G., Brahmachari, V. & Brahmachari, S. K. (2005). Comparative analysis of chromatin landscape in regulatory regions of human housekeeping and tissue specific genes. BMC Bioinformatics, 6, 126.

Sachdeva, G., Kumar, K., Jain, P. & Ramachandran, S. (2005). SPAAN: a software program for prediction of adhesins and adhesin-like proteins using neural networks. Bioinformatics, 21, 483-491.

2004

Bakshi, R., Prakash, T., Dash, D. & Brahmachari, V. (2004). In silico characterization of the INO80 subfamily of SWI2/SNF2 chromatin remodeling proteins. Biochem. Biophys. Res. Commun. 320, 197-204.

Chattopadhyay, A., Chattopadhyay, A. K. & Rao, C. B. (2004). Bhattacharyya's distance measure as a precursor of genetic distance measures. J. Biosci. 29, 135-138.

Nandi, T., Brahmachari, S. K., Kannan, K. & Ramachandran, S. (2004). Clusters of proteins in archaeal and bacterial proteomes using compositional analysis. In Silico. Biol. 4, 573-591.

Prakash, T., Khandelwal, M., Dasgupta, D., Dash, D. & Brahmachari, S. K. (2004). CoPS: Comprehensive Peptide Signature database. Bioinformatics, 20, 2886-2888.

Pandey, N., Ganapathi, M., Kumar, K., Dasgupta, D., Das Sutar, S. K. & Dash, D. (2004). Comparative analysis of protein unfoldedness in human housekeeping and non-housekeeping proteins. Bioinformatics, 20, 2904-2910.

Sharma, A., Srivastava, G. P., Sharma, V. K. & Ramachandran, S. (2004). ArrayD: a general purpose software for microarray design. BMC Bioinformatics, 5, 142.

Sharma, R., Maheshwari, J. K., Prakash, T., Dash, D. & Brahmachari, S. K. (2004). Recognition and analysis of protein-coding genes in severe acute respiratory syndrome associated coronavirus. Bioinformatics, 20, 1074-1080.

2003

Kalia, V. C., Lal, S., Ghai, R., Mandal, M. & Chauhan, A. (2003). Mining genomic databases to identify novel hydrogen producers. Trends Biotechnol. 21, 152-156.

Kalia, V. C., Chauhan, A., Bhattacharyya, G. & Rashmi (2003). Genomic databases yield novel bioplastic producers. Nat. Biotechnol. 21, 845-846.

2002

Nandi, T., Rao, C. & Ramachandran, S. (2002). Comparative genomics using data mining tools. J. Biosci. 27, 15-25.

INSTITUTE OF LIFE SCIENCES, BHUBANESWAR.

2007

Patra, M., Pandey, S.K., Ramamurthy, T., Singh, D.V. & Das, S.K. (2007). Characterization of cytotoxin producing Aeromonas caviae (strain HT10) isolated from a sulfur spring in Orissa, India. Lett. Appl. Microbiol. 44, 338-341.

Gautam, U.S., Jajoo, A., Singh, A., Chakrabartty, P.K. & Das, S.K. (2007). Characterization of a rpoN mutant of Mesorhizobium ciceri. J. Appl. Microbiol. (In press).

2006

Nataraj, S.P., Kavi Kishor, P.B., Reddy, L.A., Mondal, P., Dash, A.K., Kar, M., Mohanty, S. & Sabat, S.C. (2006). In silico modeling and hydrogen peroxide binding study of rice catalase. In Silico Biol. 6, 435-437.

Das, S. K., Gautam, U. S., Chakrabartty, P. K. & Singh, A. (2006). Characterization of a symbiotically defective serine auxotroph of Mesorhizobium ciceri. FEMS Microbiol. Lett. 263, 244-251.

INTERNATIONAL CENTRE FOR GENETIC ENGINEERING AND BIOTECHNOLOGY, NEW DELHI.

2007

Ramasamy G., Gupta D., Mohmmed A. & Chauhan V.S. (2007). Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV protease. Mol. Biochem. Parasitol. 152, 139-148.

2006

Kalita M.K., Ramasamy G., Duraisamy S., Chauhan V.S. & Gupta D. (2006). ProtRepeatsDB database of amino acid repeats in genome. BMC Bioinformatics, 7, 336.

2005

Gowthaman R., Duraisamy S., Kalita M.K. & Gupta D. (2005). A database for Plasmodium falciparum protein models. Bioinformation, 1, 50-51.

2004

Ravi Chandra B., Gowthaman R., Raj Akhouri R., Gupta D. & Sharma A. (2004). Distribution of proline-rich (PxxP) motifs in distinct proteomes: functional and therapeutic implications for malaria and tuberculosis. Protein Eng. Des. Sel. 17, 175-182.

Gajinder, P. S., Ravi, C. B., Arindam, B., Reetesh, R. A., Saurabh, K. S. & Amit, S. (2004). Hyper-expansion of asparagines correlates with an abundance of proteins with prion-like domains in Plasmodium falciparum. Mol. Biochem. Parasitol. 137, 307-319.

2003

Bahl A., Brunk B., Crabtree J., Fraunholz M., Gajria B., Grant G.R., Ginsburg H., Gupta D., Kissinger J.C., Labo P., Li L., Mailman M.D., Milgram A.J., Pearson D.S., Roos D.S., Schug J., Stoeckert Cj Jr. & Whetzel P. (2003). PlasmoDB : The Plasmodium genome resource. A database integrating experimental and computational data. Nucl. Acids Res. 31, 212-215.

2002

Kissinger J.C., Brunk B., Crabtree J., Fraunholz M., Gajria B., Milgram A.J., Pearson D.S., Schug J., Bahl A., Diskin S.J., Ginsburg H., Grant G.R., Gupta D., Labo P., Li L., Mailman M.D., McWeeney S.K., Whetzel P., Stoeckert Cj Jr. & Roos D.S. (2002). The Plasmodium genome database. Designing and mining a eukaryotic genomic resource. Nature, 3, 490-492.

Bahl A., Brunk B., Coppel R.L., Crabtree J., Diskin S.J., Fraunholz M.J., Grant G.R., Gupta D., Huestis R.L., Kissinger J.C., Labo P., Li L., McWeeney S.K., Milgram A.J., Roos D.S., Schug J. & Stoeckert CJ Jr. (2002). PlasmoDB: the Plasmodium genome resource. An integrated database providing tools for accessing, analyzing and mapping expression and sequence data (both finished and unfinished). Nucl. Acids Res. 3O, 87-90.

JAI NARAIN VYAS UNIVERSITY, JODHPUR.

2006

* Garg, A. R. & Bhaumik, B. (2006). Ratio of Average Inhibitory to Excitatory Conductance Modulates the Response of Simple Cell. Lect. Note. Comp. Sci. 4232, 82-89.

2005

* Garg, A. R., Obermayer, K. & Bhaumik, B. (2005). Development of feed-forward Receptive Field Structure of a Simple Cell and its Contribution to the Orientation Selectivity: A Modelling Study. Int. J. Neural Syst. 15, 55-70.

* Garg, A. R., Bhaumik, B. & Obermayer, K. (2005). Variable Discharge Pattern and Contrast Invariant Orientation Tuning of a Simple Cell: A Modelling Study. Neural Inf. Proc. Lett. Rev., 6, 59-68.

2002

* Bhaumik, B. & Garg, A. R. (2002). Direction-selective simple cells in cat striate cortex: a developmental mode. Neural Net. 1, 778 –783.

JAWAHARLAL NEHRU UNIVERSITY, NEW DELHI.

2007

Thakur, V., Azad, R. K. & Ramaswamy, R. (2007). Markov models of Genome segmentation. Phys. Rev. E, 75, 011915.

Srivastava, P. K., Desai, D. K., Nandi, S. & Lynn, A. M. (2007). HMM-ModE - Improved classification using profile hidden Markov models by optimising the discrimination threshold and modifying emission probabilities with negative training sequences. BMC Bioinformatics, 8, 104.

Vishnoi, A., Roy, R. & Bhattacharya, A. (2007). Comparative analysis of Bacterial genomes: Identification of divergent regions in Mycobacterial strains using an anchor-based approach. Nucl. Acid Res. (In press).

2006

Mandal, P.K., Rawal, K., Ramaswamy, R., Bhattacharya, A. & Bhattacharya, S. (2006). Identification of insertion hot spots for non-LTR retrotransposons: computational and biochemical application to Entamoeba histolytica. Nucl. Acids Res. 34, 5752-5763.

Haimovich, A. D., Byrne B., Ramaswamy R. & Welsh, W. J. (2006). Wavelet Analysis of DNA Walks. J. Comput. Biol. 13, 1289-1298.

Mehra, A., Fredrick, J., Petri, W. A. Jr, Bhattacharya, S. & Bhattacharya, A. (2006). Expression and function of a family of transmembrane kinases from the protozoan parasite Entamoeba histolytica. Infect. Immun. 74, 5341-5351.

Bhattacharya, A., Padhan, N., Jain, R. & Bhattacharya, S. (2006). Calcium-binding proteins of Entamoeba histolytica. Arch. Med. Res. 37, 221-225.

Pandey, S. P. & Krishnamachari A. (2006). Computational analysis of plant RNA Pol-II promoters. BioSystems, 83, 38-50.

Pareek, A., Singh, A., Kumar, M., Kushwaha, H. R., Lynn, A. M. & Singla-Pareek, S. L. (2006). Whole-genome analysis of Oryza sativa reveals similar architecture of two-component signaling machinery with Arabidopsis. Plant Physiol. 142, 380-397.

2005

Gourinath, S., Padhan, N., Alam N. & Bhattacharya, A. (2005). Crystallization and preliminary crystallographic analysis of calcium-binding protein-2 from Entamoeba histolytica and its complexes with strontium and the IQ1 motif of myosin V. Acta Cryst. F61, 417-420.

Loftus, B., Anderson, I., Davies, R., Alsmark, U. C., Samuelson, J., Amedeo, P., Roncaglia, P., Berriman, M., Hirt, R. P., Mann, B. J., Nozaki, T., Suh, B., Pop, M., Duchene, M., Ackers, J., Tannich, E., Leippe, M., Hofer, M., Bruchhaus, I., Willhoeft, U., Bhattacharya, A., Chillingworth, T., Churcher, C., Hance, Z., Harris, B., Harris, D., Jagels, K., Moule, S., Mungall, K., Ormond, D., Squares, R., Whitehead, S., Quail, M. A., Rabbinowitsch, E., Norbertczak, H., Price, C., Wang, Z., Guillen, N., Gilchrist, C., Stroup, S. E., Bhattacharya, S., Lohia, A., Foster, P. G., Sicheritz-Ponten, T., Weber, C., Singh, U., Mukherjee, C., El-Sayed, N. M., Petri, W. A. Jr., Clark, C. G., Embley, T. M., Barrell, B., Fraser, C. M., Hall, N. (2005). The genome of the protist parasite Entamoeba histolytica. Nature, 433, 865-868.

Nandi, S., Mehra, N., Lynn, A. M., Bhattacharya, A. (2005). Comparison of theoretical proteomes: Identification of COGs with conserved and variable pI within the multimodal pI distribution. BMC Genomics, 6, 116.

Vats, D., Vishwakarma, R. A., Bhattacharya, S., Bhattacharya, A. (2005) Reduction of cell surface glycosylphosphatidylinositol conjugates in Entamoeba histolytica by antisense blocking of E. histolytica GlcNAc-phosphatidylinositol deacetylase expression: effect on cell proliferation, endocytosis, and adhesion to target cells. Infect. Immun. 73, 8381-8392.

Bakre, A. A., Rawal, K., Ramaswamy, R., Bhattacharya, A. & Bhattacharya, S. (2005). The LINEs and SINEs of Entamoeba histolytica: comparative analysis and genomic distribution. Exp Parasitol. 110, 207-213.

Bansal-Mutalik, R., Mustafi, S. M., Bhattacharya, A. & Chary, K. V. (2005). Sequence specific 1HN, 13C and 15N resonance assignments of a novel calcium-binding protein from Entamoeba histolytica. J. Biomol. NMR. 31, 379-380.

Deswal, R., Singh, R., Lynn, A. M. & Frank, R. (2005). Identification of immunodominant regions of Brassica juncea glyoxalase I as potential antitumor immunomodulation targets. Peptides, 26, 395-404.

Sharma, P., Sahni, N. S., Tibshirani, R., Skaane, P., Urdal, P., Berghagen, H., Jensen, M., Kristiansen, L., Moen, C., Sharma, P., Zaka, A., Arnes, J., Sauer, T., Akslen, L. A., Schlichting, E., Borresen-Dale, A. L. & Lonneborg. A. (2005). Early detection of breast cancer based on gene-expression patterns in peripheral blood cells. Breast Cancer Res. 7, R634-R644.

Sahni, N. S., Isaksson, T. & Naes, T. (2005). Comparison of methods for transfer of calibration models in near-infared spectroscopy: a case study based on correcting path length differences using fiber-optic transmittance probes in in-line near-infrared spectroscopy. Appl. Spectrosc. 59, 487-495.

Agarwal, S. M. (2005). Evolutionary rate variation in eukaryotic lineage specific human intronless proteins. Biochem. Biophys. Res. Commun. 337, 1192-1197.

Agarwal, S. M. & Gupta, J. (2005). Comparative analysis of human intronless proteins. Biochem. Biophys. Res. Commun. 331, 512-519.

2004

Mandal, P. K., Bagchi, A., Bhattacharya, A. & Bhattacharya, S. (2004). An Entamoeba histolytica LINE/SINE pair inserts at common target sites cleaved by the restriction enzyme-like LINE-encoded endonuclease. Eukaryot. Cell, 3, 170-179.

Chakrabarty, P., Sethi, D. K., Padhan, N., Kaur, K. J., Salunke, D. M., Bhattacharya, S. & Bhattacharya, A. (2004). Identification and characterization of EhCaBP2. A second member of the calcium-binding protein family of the protozoan parasite Entamoeba histolytica. J. Biol. Chem. 279, 12898-12908.

Krishnamachari, A., Moy Mandal, V. & Karmeshu. (2004). Study of DNA binding sites using the Renyi parametric entropy measure. J. Theor. Biol. 227, 429-436.

* Sharma, D., Issac, B., Raghava, G. P. & Ramaswamy, R. (2004). Spectral Repeat Finder (SRF): identification of repetitive sequences using Fourier transformation. Bioinformatics, 20, 1405-1412.

* Singh, B.K., Subba Rao, J., Ramaswamy, R. & Sinha, S. (2004). The role of heterogeneity on the spatiotemporal dynamics of host-parasite metapopulation. Ecolo. Model. 180, 435-443.

2003

Satish, S., Bakre, A. A., Bhattacharya, S. & Bhattacharya, A. (2003). Stress-dependent expression of a polymorphic, charged antigen in the protozoan parasite Entamoeba histolytica. Infect. Immun. 71, 4472-4486.

Bhattacharya, A., Bhattacharya, S. & Ackers, J. P. (2003). Nontranslated polyadenylated RNAs from Entamoeba histolytica. Trends Parasitol. 19, 286-289.

Ghosh, S,, Satish, S., Tyagi, S., Bhattacharya, A. & Bhattacharya, S. (2003). Differential use of multiple replication origins in the ribosomal DNA episome of the protozoan parasite Entamoeba histolytica. Nucl. Acids Res. 31, 2035-2044.

Jha, S., Karnani, N., Lynn, A. M. & Prasad, R. (2003) Covalent modification of cysteine 193 impairs ATPase function of nucleotide-binding domain of a Candida drug efflux pump. Biochem. Biophys. Res. Commun. 310, 869-875.

2002

Bhattacharya, S., Bakre, A. & Bhattacharya, A. (2002). Mobile genetic elements in protozoan parasites. J. Genet. 81, 73-86.

Azad, R.K., Subba Rao, J., Li, W. & Ramaswamy, R. (2002). Simplifying the mosaic description of DNA sequence. Phys. Rev. E66, 031913.

Azad, R.K., Pernola-Galvan, P., Ramaswamy, R. & Subba Rao, J. (2002). Segmentation of Genomic DNA through entropic divergenceL Power laws and Scaling. Phys. Rev. E65, 051909.

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2007

* Malathi, S., Karunasagar, I. & Karunasagar, I. (2007). Abundance, composition and distribution of simple sequence repeats and dinucleotide compositional bias within WSSV genomes. Ind. J. Genet. (In press).

* Rekha, K., Malathi, S., Indrani, K. & Karunasagar, I. (2007). A bioinformatic based study of OmpTS protein of Aeromonas hydrophila : a potential vaccine candidate for aquaculture. Aquaculture (In press).

2006

* Godhe, A., McQuoid, M.R., Karunasagar, I., Karunasagar, I. & Rehnstam, H. A. S. (2006). Comparison of three common molecular tools for distinguishing among geographically separated clones of the diatom Skeletonema marinoi sarno et zingone (Bacillariophyceae). J. Phycol. 42, 280-291.

Parvathi, A., Sanath, K. H., Karunasagar, I. & Karunasagar, I. (2005). Study of occurrence of V. vulnificus by RAPD and gyrB sequence analysis. Environ. Microbiol. 7, 995-1002.

* Malathi, S., Karunasagar, I. & Karunasagar, I. (2005). A computer based identification of variable number of tandem repeats in White Spot Syndrome Virus (WSSV) genomes. Curr. Sci. 89, 882-887.

Manjanaik, B., Umesha, K.R., Karunasagar, I. & Karunasagar, I. (2005). Detection of hepatopancreatic parvovirus (HPV) in wild shrimps in India by nested polymerase chain reaction (PCR). DAO. 63, 255-259.

2004

Manivannan, S., Bob, K.M.D., Karunasagar, I. & Karunasagar, I. (2004). Prevalence of monodon baculovirus (MBV) in wild Metapenaeus species along the south west coast of India. Aquaculture, 232, 63-67.

2003

* Dhanashree, B., Otta, S.K., Karunasagar, I., Goebel, W. & Karunasagar, I. (2003). Incidence of Listeria spp. in clinical and food samples in Mangalore, India. Food Microbiol. 20, 447-453.

* Dhanashree, B., Otta, S.K., Karunasagar, I. & Karunasagar, I. (2003). Protein profile analysis of Listeria monocytogenes strains from tropics. Curr. Sci. 84, 628-630.

Karunasagar, I., Rivera, B., Joseph, B., Kennedy, V.R., Shetty, A., Huq, I., Karunasagar, I. & Colwell R.R. (2003). OmpU genes in nontoxigenic Vibrio cholerae associated with aquaculture. J. Appl. Microbiol. 95, 338-343.

2002

* Chakraborty, A., Otta, S.K., Joseph, B., Sanath, K.H., Shahadat, H. Md.., Karunasagar I., Venugopal, M.N. & Karunasagar I. (2002). Prevalence of white spot syndrome virus (WSSV) in wild crustaceans along the coast of India. Curr. Sci. 82, 1392-1397.

* Manivannan, S., Otta, S.K., Karunasagar, I. & Karunasagar, I. (2002). Multiple viral infection in Penaeus monodon shrimp postlarvae in an Indian hatchery. DAO. 48, 233-236.

MADRAS UNIVERSITY, CHENNAI.

2007

* Gowri, S. B. A., Sarani, R., Daliah, M., Mridula, P., Vasuki, R. C., Sowmiya, G., Vasundhar, G., Sudha, P., Jayakanthan, J., Velmurugan, D. & Sekar, K. (2007). Ion pairs in non-redundant protein structures. J. Biosci. 32, 693-704.

Kanagasabai, V., Arunachalam, J., Arun, P. P. & Gautham, N (2007). Exploring the conformational space of protein loops using a mean field technique with MOLS sampling. Proteins: Struct. Funct. Bioinformatics (In Press).

Malathy, S. S. M. & Ponnuswamy, M. N. (2007). Molecular basis behind the substrate specificity of Polygalacturonase through computational study. Polymer, 48, 910-916.

Sreekanth, R. & Rajan, S. S. (2007). The study of helical distortions due to environmental changes: Choice of parameters. Biophys. Chem. 125, 191-200.

2006

Arunachalam, J., Kanagasabai, V. & Gautham, N. (2006). Protein Structure Prediction Using Mutually Orthogonal Latin Squares and a Genetic Algorithm. Biophys. Biochem. Res. Commun. 342, 424-433.

Bharanidharan, D. N. & Gautham, N. (2006). Principal Component Analysis (PCA) of DNA Oligonucleotide Structural Data. Biophys. Biochem. Res. Commun. 340, 1229-1237.

* Jayalakshmi, J., Mridula, P., Sekar, K., Vaijayanthimala, S. & Velmurugan, D. (2006). Interaction of water molecules in non-identical protein structures. Ind. J. Chem. 45A, 159-162.

Malathy, S. S. M., Saraboji, K., Sukumar, N. & Ponnuswamy, M. N. (2006). Role of amino acid properties to determine backbone $\tau(\text{N-C}\alpha\text{-C}')$ stretching angle in peptides and proteins. Biophys. Chem. 12O, 24-31.

Malathy, S. S. M. & Ponnuswamy, M. N. (2006). Nature of $\prod$-Interactions in nitrogen-containing heterocyclic systems: A structural database analysis. Cryst. Growth Des. (In Press).

OmPraba, G. & Velmurugan, D. (2006). Quantitative structure-activity relationship (QSAR) analysis of a series of indole analogues as inhibitor for human group V secretory phospholipase A2. Ind. J. Biochem. Biophys. 43. (In Press).

Saraboji, K., Gromiha, M. M. & Ponnuswamy, M. N. (2006). Average assignment method for predicting the stability of protein mutants. Biopolymers (In Press).

Thiyagarajan, S., Rajan, S. S. & Gautham, N. (2006). Effect of DNA structural flexibility on promoter strength – Molecular dynamics studies of E. coli promoter sequences. Biophys. Biochem. Res. Commun. 341, 557-566.

2005

Arun, P. P., Vengadesan, K. & Gautham, N. (2005). MOLS - A program to explore the potential energy surface of a peptide and locate its low energy conformations. In Silico Biol. 5, 401-405.

Bharanidharan, D. & Gautham, N. (2005). Amino acid variation in cellular processes in 108 bacterial proteomes. Arch. Microbiol. 184, 168-174.

Saraboji, K., Gromiha, M. M. & Ponnuswamy, M. N. (2005). Relative importance of secondary structure and solvent accessibility to the stability of protein mutants: A case study with amino acid properties and energetics on T4 and human lysozymes. Comp. Biol. Chem. 29, 25-35.

Saraboji, K., Gromiha, M. M. & Ponnuswamy, M. N. (2005). Importance of main-chain hydrophobic free energy to the stability of thermophilic proteins. Int. J. Biol. Macromol. 35, 211-220.

Vengadesan, K. & Gautham, N. (2005). A new conformational search technique and its applications. Curr. Sci. 88, 1759-1770.

Thenmalarchelvi, R. & Yathindra, N. (2005). New insights into DNA triplexes: Residual twist and radial difference as measures of base triplet non-isomorphism and their implication to sequence-dependent non-uniform DNA triplex. Nucl. Acids Res. 33, 43-55.

2004

Bharanidharan, D., Bhargavi, G. R., Uthanumallian, K. & Gautham, N. (2004). Correlations between nucleotide frequencies and amino acid composition in 115 bacterial species. Biochem. Biophys. Res. Commun. 315, 1097-1103.

Nallini, A., Saraboji, K. & Ponnuswamy, M. N. (2004). A study of aromatic hydrogen bonds for peptides with aromatic amino acid side-chains. Ind. J. Biochem. Biophys. 41, 184-187.

Vengadesan, K. & Gautham, N. (2004). Conformational studies on enkephalins using the MOLS technique. Biopolymers, 74, 476-494.

Vengadesan, K., Anbupalam, T. & Gautham, N. (2004). An application of experimental design using mutually orthogonal Latin squares in conformational studies of peptides. Biochem. Biophys. Res. Commun. 316, 731-737.

Vengadesan, K. & Gautham, N. (2004). Energy landscape of met-enkephalin and leu-enkephalin drawn using mutually orthogonal Latin square sampling. J. Phy. Chem. B108, 11196-11205.

2003

Ramya, B. G., Sheik S. S., Velmurugan, D. & Sekar, K. (2003). Side-chain conformation angles of amino acids: effect of temperature factor cut-off. J. Struct. Biol. 143, 181-184.

Thenmalarchelvi, R. & Yathindra, N. (2003). Residual hoogsteen twist as a measure of non-isomorphism in DNA. Base triplets Implication to sequence dependent DNA triplexes. Rec. Trends Bio. Res. 17-24.

Vengadesan, K. & Gautham, N. (2003). Enhanced sampling of the molecular potential energy surface using mutually orthogonal Latin squares: application to peptide structures. Biophys J. 84, 2897-2906.

2002

Premraj, B. J., Raja, S. & Yathindra, N. (2002). Structural basis for the unusual properties of 2', 5' nucleic acids and their complexes with RNA and DNA. Bio.Phy.Chem. 95, 253-272.

MADURAI KAMARAJ UNIVERSITY, MADURAI.

2007

Singh, S. K., Dessalew, N., & Bharatam, P. V. (2007). 3D-QSAR CoMFA Study on Oxindole Derivatives as Cyclin Dependent Kinase 1 (CDK1) and Cyclin Dependent Kinase 2 (CDK2) Inhibitors. Med. Chem. 3, 75-84.

Dessalew, N., Singh, S. K. & Bharatam, P. V. (2007). 3D-QSAR CoMFA Study on Aminothiazole Derivatives as Cyclin Dependent Kinase 2 Inhibitors. QSAR Comb. Sci. 26, 85-91.

Singh, S. K. & Sundar Ram, N. (2007). Theoretical Studies on Cyclin Dependent Kinase (CDK4) Inhibitors and drug receptor interaction analysis. Med. Chem. Res. 15, 367-369.

Gopal, P., Pravin Kumar, P., Sinilal, B, Jose, J ., Kasin Y. & Usha, R. (2007). Differential roles of C4 and βC1 in mediating suppression of posttranscriptional gene silencing: Evidence for transactivation by the C2 of Bhendi yellow vein mosaic virus, a monopartite begomovirus. Virus Res. 123, 9-18.

Vadivukarasi,T., Girish, K.R. & Usha, R. (2007) Sequence and recombination analysis of the replication initiator protein. J. Biosciences, 32, 17-29.

Srividhya, K.V. & Krishnaswamy, S. (2007) Sub classification and targeted characterization of prophage encoded two-component cell lysis cassette. J. Biosciences, 32. (In press)

Palanivelu, P. (2007). Multiple sequence analysis of polygalacturonases and invertases and phase shift in conserved motifs. Indian J. Biotechnol. 6, 24-30.
Avi, Z., Pravin, P. K., Usha, R., Yael, L., Abraham, L., Tzahi, A., Moshe, L. & Yedidya, G. (2007). Production of siRNA targeted against TYLCV coat protein transcripts leads to silencing of its expression and resistance to the virus. Trans. Res. 16, 385-398.

2006

Sridhar, J. and Rafi, Z.A. (2006). Small RNA identification in Enterobacteriaceae using synteny and genomic backbone retention. OMICS: A Journal of Integrative Biology, 11 , 74-95.

Singh, S. K., Dessalew, N. & Bharatam, P. V. (2006). 3D-QSAR CoMFA studies on Indenopyrazole as CDK2 Inhibitors. Eur. J. Med. Chem. 41, 1310-1319.

Srividhya, K. V., Geeta, V. R., Raghavenderan, L., Preeti, M., Jaime, P., Sankarnarayanan, M., Joel, L. S. & Krishnaswamy, S. (2006). Database and Comparative Identification of Prophages. In ICIC 2006, LNCIS D.-S. Huang, K. Li, and G.W. Irwin (Eds.), Springer-Verlag, 344, 863 – 868.

Jeyakumar, N., Daniel, B., Werner, D., Catherine, H., Yonghong, Z., Catherine, D., James, R. V. B. & Eric, G. B. (2006). Text mining of full-text journal articles combined with gene expression analysis reveals a relationship between sphingosine-1-phosphate and invasiveness of a glioblastoma cell. BMC Bioinformatics, 7, 373.

Sundara, B. N., Mathew, M. K. & Krishnaswamy, S. (2006). Functional assay of S.typhi OmpC using reconstituted large unilamellar vesicles: A general method for characterization of outer membrane proteins. Biochimie. 88, 1419-1424.

Girish, K. R., Palanivelu, S., Kumar, P. D. & Usha, R. (2006). Refolding, purification and characterization of replication-initiator protein from soybean-infecting geminivirus. J. Virol. Meth. 136, 154-159.

Pravin Kumar, P., Usha, R., Zrachya, A., Levy, Y., Spanov, H. & Gafni, Y. (2006). Protein–protein interactions and nuclear trafficking of coat protein and βC1 protein associated with Bhendi yellow vein mosaic disease. Virus Res. 122, 127-136.

Shivaprasad, P.V., Thillaichidambaram, P., Balaji, V. & Veluthambi, K. (2006). Expression of full-length and truncated Rep genes from Mungbean yellow mosaic virus-Vigna inhibits viral replication in transgenic tobacco. Virus Genes, 33, 365-374.

Palanivelu, P. (2006). Polygalacturonases: Active site analyses and Mechanism of action. Indian J. Biotechnol. 5, 148-162.

2005

Uma, M., Anton, M., Johannes, G., Krishnasamy, S., Rajyashri, Villoo, M. P., K. R. & Chris, B. (2005). The Diatom EST Database. Nucl Acids Res. 33, D344-D347.

* Rajeshwari, M. & Palanivelu, P. (2005). UlTRaSCAN - an algorithm for prediction of pattern (s) in untranslated regions of eukaryotic mRNAs. Indian J. Biotechnol. 4, 21-38.

Kumar, P. D. & Krishnaswamy, S. (2005). Overexpression, refolding, and puri.cation of the major immunodominant outer membrane porin OmpC from Salmonella typhi: characterization of refolded OmpC. Protein Expr. Purif. 40, 126-133.

Yadav, A. & Singh, S. K. (2005). Common binding mode for structurally and chemically diverse non-nucleosidic HIV-1RT inhibitors. J. Mol. Struct.(Theochem). 723, 205-209.

Shabaana, A. K., Kulangar, K., Semac, I., Parel, Y.,Ilangumaran, S., Dharmalingam, K., Chizzolini, C. & Hoessli, D. C. (2005). Mycobacterial liporaabinomannans modulate cytokine production in human T helper cells by interfering with raft/microdomain signaling. Cell. Mol. Life Sci. 62, 001-009.

Girish, K. R. & Usha, R. (2005). Molecular characterization of two soybean infecting begomoviruses from India and evidence for recombination among legume infecting begomoviruses from South-East Asia. Virus Res. 108, 167-176.

Shivaprasad, P. V., Akbergenov, R., Trinks, D., Rajeswaran, R., Veluthambi, K., Hohn, T. & Pooggin, M. M. (2005). Promoters, transcripts and regulatory proteins of mungbean yellow mosaic geminivirus. J. Virol. 79, 8149-8160.

Natarajan J, Berrar D, Hack C.J, Dubitzky W. (2005). Knowledge Discovery in Biology and Biotechnology Texts: A Review of Techniques, Evaluation Strategies, and Applications. Crit. Rev. Biotechnol. 25, 31-52.

Ramachandran, S. S., Shunmugiah, K. P., Nirmala Lini, Abdul Khader Shabaana, Nagavardhini, A. & Dharmalingam, K. (2005). Cloning of mce1 locus of Mycobacterium leprae in Mycobacterium smegmatis mc2 155 SMR5 and evaluation of expression of mce1 genes in M. smegmatis and M. leprae. FEMS Immunol. Med. Microbiol. 45, 291-302.

* Rajeshwari, M. & Palanivelu, P. (2005) UlTRaSCAN - an algorithm for prediction of pattern (s) in untranslated regions of eukaryotic mRNAs. Indian J. Biotechnol. 4, 21-38.

Guerra-Peraza, O., Kirk, D., Seltzer, V., Veluthambi, K., Schmidt, A. C. Hohn, T. & Herzog, E. (2005). Coat proteins of Rice tungro bacilliform virus and Mungbean yellow mosaic virus contain multiple nuclear-lacalization signals and interact with importin α. J. Gen. Virol. 86, 1815-1826.

Sundara, B. N., Ravi, A. K., Singh, T. P. & Krishnaswamy, S. (2005). High-resolution diffraction from crystals of a membrane protein complex: bacterial Outer Membrane Protein, OmpC with antibacterial eukaryotic protein, Lactoferrin. Acta Cryst. F61, 773-775.

Preeti, M., Krishnamohan, K. & Krishnaswamy, S. (2004). HNH family sub-classification leads to identification of commonality in the His-Me endonuclease superfamily. Protein Sci. 13, 295-300.

Preeti, M., Casjens, S. & Krishnaswamy, S. (2004). Analysis of the lambdoid prophage element e14 in the E.coli K-12 genome. BMC Microbiol. 4, 4.

Arockiasamy, A., Murthy, G. S., Rukmini, M. R., Sundara Baalaji, N., Umesh, C. K. & Krishnaswamy, S. (2004). Conformational epitope mapping of OmpC, a major cell surface antigen from Salmonella typhi. J. Struct. Biol. 148, 22-33.

Arockiasamy, A., Kumar, P. D., Sundara Baalaji, N., Rukmini, M. R. & Krishnaswamy, S. (2004). Folding and structural stability of OmpC from Salmonella typhi: Role of LPS and environment. Curr. Sci. 87, 197-202.

Mohan Katta, A. V. S. K., Rajeshwari, M., Rajiv V. B. & Krishnaswamy, S. (2004). Consensus based validation of membrane porins. In silico biol. 4, 549-561.

Srividhya, K. V. & Krishnaswamy, S. (2004). A simulation model of Escherichia coliosmoregulatory switch using E-CELL system. BMC Microbiol. 4, 44.

Yadav, A. & Singh, S. K. (2004). Threshold interaction energy of NRTI's (2'-deoxy 3'-substituted nucleosidic analogs of Reverse transcriptase) to undergo competitive inhibition. Bioorg. Med. Chem. lett. 14, 2677-2680.

Banerjee, G., Damodaran, A., Devi, N., Dharmalingam, K. & Raman, G. (2004). Role of Keratinocytes in Antigen Presentation and Polarization of Human T Lymphocytes. Scand. J. Immunol. 59, 385-394.

Karthikeyan, A. S., Vanitharani, R., Balaji, V., Anuradha, S., Thillaichidambaram, P., Shivaprasad, P. V., Parameswari, C., Balamani, V., Saminathan, M. & Veluthambi, K. (2004). Analysis of an isolate of Mungbean yellow mosaic virus (MYMV) with a highly variable DNA B component. Arch. Virol. 149, 1643-1652.

Kanagavalli, J., Eswari, P., Subbaiah, R. K., Krishnaswamy, S. & Sundaresan, P. (2004). A Review of Genetic and Structural Understanding of the Role of Myocilin in Primary Open Angle Glaucoma. Indian J. Ophthalmol. 52, 271-280.

2003

Vasanthi, G., & Krishnaswamy, S. (2003). Dipole moment in TIM alpha/beta fold proteins. Ind. J. Biochem. Biophys. 40, 194-202.

Kanagavalli, J., Subbaiah, R. K., Eswari, P., Krishnaswamy, S. & Periasamy, S. (2003). Evaluation and understanding of myocilin mutations in Indian primary open angle glaucoma patients. Mol. Vis. 9, 606-614.

Paranthaman, S., & Dharmalingam, K. (2003). Intergeneric Conjugation in Streptomyces peucetius and Streptomyces sp. strain C5: Chromosomal integration and expression of recombinant plasmids carrying chiC gene. Appl. Environ. Microbiol. 69, 84-91.

Shabaana, A. K., Shanker Narayan, N. P. and Dharmalingam, K. (2003) M. leprae 18-kDa Heat shock protein gene is polymorphic. Curr. Sci. 84, 64-70.

Daisy Vanitha, J., Venkatasubramani, R., Dharmalingam, K. & Paramasivan, C. N. (2003). Large – Restriction – Fragment Polymorphism analysis of Mycobacterium chelonae and Mycobacterium terrae isolates. Appl. Environ. Microbiol. 69, 4337-4341.

Jacob, T., Jebasingh, T., Venugopal, M. N. & Usha, R. (2003). High genetic diversity in the coat protein and the 3'untranslated regions among the geographical Isolates of Cardamom mosaic virus from south India. J. Biosci. 28, 589-595.

Ranjan Prasad, Sasikala, V., Vetrivel, K. S. and Dharmalingam, K. (2003). A novel extracellular protein of Streptomyces peucetius binds to daunorubicin but does not inhibit the bioactivity of the antibiotic. Biochem. Biophys. Res. Commun. 311, 460-464.

Jose, J. & Usha, R. (2003). Bhendi Yellow Vein Mosaic Disease in India Is Caused by Association of a DNA Beta Satellite with a Begomovirus. Virology, 305, 310-317.

2002

Vasanthi, G. & Krishnaswamy, S. (2002). Dipole moment analysis of membrane proteins suggests role in orientation in the membrane. Ind. J. Biochem. Biophys. 39, 93-100.

Jacob, T. & Usha, R. (2002). Expression of Cardamom mosaic virus coat protein in Escherichia coli and its assembly into filamentous aggregates. Virus Res. 86, 133-141.

NATIONAL BRAIN RESEARCH CENTRE,

2007

Joti, P., Kulashekhar, S., Behari, M. & Murthy, A. (2007). Impaired inhibitory oculomotor control in patients with Parkinson's disease. Exp. Brain Res. 177, 447-457.

Singh, L. & Singh, N.C. (2007) The development of articulatory signatures in children, Developmental Science (in press).

Tanusree, D., Latika, S. & Nandini, C. S. (2007). Rhythmic structure of English and Hindi – new insights from a computational analysis. Prog. Brain Res. (in press).

Murthy, A., Ray, S., Stephanie, M. S., Elizabeth, G. P., Schall, J.D. & Thompson, K. G. (2007). Frontal eye field contributions to rapid corrective saccades. J. Neurophysiol. 97, 1457-1469.

Singh, L., Shantisudha, P. & Singh, N. C. (2007). Developmental patterns of speech in children. J. Appl. Acoustics 68, 260-268.

2004

Ray, S., Schall, J. D. & Murthy, A. (2004). Programming of double step saccade sequences: Modulation by cognitive control. Vision Research, 44, 2271-2707.

Roy, P. (2004). Stochastic Resonance Imaging and Stochastic Resonance Therapy: preliminary studies considering the brain as stochastic processor. Lect. Note. Comp. Sci. 3316, 96-103.

Roy, P. (2004). Stochastic Resonance as an Emerging Technique for Neuromodulation: Using Nonlinear Dynamics to Analyze EEG and Drug-induced Language Transition. J. Quant. Ling. 11, 47-77.

2003

Roy, P. (2003). Cognitive Processing: An Analysis using Stochastic Activation. J. Inst. Elect. Telecom. Eng. 49, 183-195.

Murthy, A. (2003). Neural control of eye movements. J. Inst. Elect. Telecom. Eng. 49, 135-144

2002

Roy, P. K., Kozman, R. & Majumder, D. D. (2002). Neurocomputation model and algorithm for phase transition and instability. IEEE Trans. Evol. Comput. 5, 1-14.

Joti, P., Kulashekhar, S., Behari, M. & Murthy, A. Impaired inhibitory oculomotor control in patients with Parkinson's disease. Exp. Brain Res. 177, 447-57

NATIONAL INSTITUTE OF PHARMACEUTICAL EDUCATION AND RESEARCH, PUNJAB.

2007

Garg, P., Verma, J. & Roy, N. (2007). In Silico Modeling for Blood Brain Barrier Permeability Predictions in Preclinical Biopharmaceutics - in situ, in vitro, and in silico tools for drug absorption studies ed Carsten Ehrhardt and Kwang-Jin (In press).

Kadam, R. U., Shivange, A. V. & Roy, N. (2007). E. coli vs P. aeruginosa deacetylase LpxC inhibitors Selectivity: Surface and Cavity depth based analysis. J. Chem. Info. Mod. (In press).

Kadam, R. U., Garg, D., Chavan, A. & Roy, N. (2007). Evaluation of Pseudomonas aeruginosa deacetylase LpxC inhibitory activity of dual PDE4-TNF ? inhibitors: A multi-screening approach. J. Chem. Info. Mod. (In press).

Kadam, R. U., Chavan, A. & Roy, N. (2007). Pharmacophoric features of Pseudomonas aeruginosa deacetylase LpxC inhibitors: An electronic and structural analysis. Bioorg. Med. Chem. Lett. 17, 861-868.

Deswal, S. & Roy, N. (2007). A novel range based QSAR study of human neuropeptide Y (NPY) Y5 receptor inhibitors. Eur. J. Med. Chem. 42, 463-470.

2006

Kadam, R. U., Kiran, V. M. & Roy, N. (2006). Comparative protein modeling and surface analysis of Leishmania sirtuin: A potential target for antileishmanial drug discovery. Bioorg. Med. Chem. Lett. 16, 6013-6018.

Kadam, R. U. & Roy, N. (2006). Cluster analysis and 2-Dimensional Quantitative Structure Activity Relationship (2D-QSAR) of Pseudomonas aeruginosa Deacetylase LpxC inhibitors. Bioorg. Med. Chem. Lett. 16, 5136-5143

Deswal, S. & Roy, N. (2006). Quantitative structure activity relationship studies of aryl heterocycle-based thrombin inhibitors. Eur. J. Med. Chem. 41, 1339-1346.

Deswal, S. & Roy, N. (2006). Quantitative Structure Activity Relationship of Benzoxazinone Derivatives as Neuropeptide Y Y5 Receptor Antagonists. Eur. J. Med. Chem. 41, 552-557

MAHATMA GANDHI INSTITUTE OF MEDICAL SCIENCE, SEVAGRAM.

2005

Deshmukh, P., Jumde, J., Kumar, S., Reddy, M. V. R. & Harinath, B. C. FilaDB - Database software for information storage and retrieval on detection and management of filaria patients. Bioinformatics India. 3, 36-46.

MANONMANIAM SUNDARANAR UNIVERSITY, TIRUNELVELI.

2006

Jeya, S. S. D. & Veluraja, K. (2006). Conformations of higher gangliosides and their binding with cholera toxin – Investigation by molecular modelling, molecular mechanics and molecular dynamics. J. Biomol. Struct. Dyn. 23, 641-656.

2005

Veluraja, K. & Margulis, C. J. (2005). Conformational dynamics of sialyl Lewisx in aqueous solution and its interaction with SelectinE – A study by Molecular Dynamics. J. Biomol. Struct. Dyn. 23, 101-111.

2004

Jeya, S. S. D. & Veluraja, K. (2004). Monosialogangliosides and their interaction with cholera toxin – Investigation by molecular modelling and molecular mechanics. J. Biomol. Struct. Dyn. 21, 591-613.

Jeya, S. S. D. & Veluraja, K. (2004). Disialogangliosides and their interaction with cholera toxin – Investigation by molecular modelling, molecular mechanics and molecular dynamics. J. Biomol. Struct. Dyn. 22, 299-313.

2003

Xavier, S. M. & Veluraja, K. (2003). Conformations of terminal sialyloligosaccharide fragments - A molecular dynamics study. J. Theor. Biol. 222, 389-402.

2002

Swaminathan, G. J., Holloway, D. E., Veluraja, K. & Acharya, K. R. (2002). Atomic Resolution (0.98A) Structure of Eosinophil Derived Neurotoxin. Biochemistry, 41, 3341-3352.

NATIONAL CENTRE FOR BIOLOGICAL SCIENCES, BANGALORE.

2007

Pugalenthi, G., Suganthan, P. N., Sowdhamini, R. & Chakrabarti, S. (2007). SMotif: A server for structural motifs in proteins. Bioinformatics (In press).

Ajay, S.M. & Bhalla, U.S. (2007). A propagating ERKII switch forms zones of elevated dendritic activation correlated with plasticity. HFSP J. (In press).

Cannon, R. C., Gewaltig, M. O., Bhalla, U. S., Cornelis, H., Gleeson, P., Hines, M. L., Howell, F. W., Muller, E., Stiles, J. R. Wils, S. & De Schutter, E. (2007). Interoperability of neuroscience modeling software: current status and future directions. Neuroinformatics, 5. (In press).

2006

Khajamohiddin, S., Babu, P. S., Chakka, D., Merrick, M., Bhaduri, A., Sowdhamini, R. & Siddavattam, D. (2006). A novel meta-cleavage product hydrolase from Flavobacterium sp. ATCC27551. Biochem. Biophys. Res. Commun. 351, 675-681.

Gadkari, R.A., Sandhya, S., Sowdhamini, R. & Dighe, R.R. (2006). The antigen binding sites of various hCG monoclonal antibodies show homology to different domains of LH receptor. Mol. Cell. Endocrinol. 351, 675-81.

Tripathi, L.P. & Sowdhamini, R. (2006). Cross-genome comparisons of serine proteases in Arabidopsis & rice. BMC Genomics, 7, 200.

Chakrabarti, S., Manohari, G., Pugalenthi, G. & Sowdhamini, R. (2006). SSToSS: Sequence Structural Templates of Single-member superfamilies. In Silico Biol. 6, 311-319.

Chandrashekar, C., Manonmani, A., Babu, M. & Sowdhamini, R. (2006). Enhanced structure prediction of gene products containing adenylyl cyclase. In Silico Biol. 6, 351-362.

* Rhana, B., Sandhya, S., Abhinandan, K.R., Chakrabarti S, Sowdhamini, R. & Srinivasan, N. (2006). Cascade PSI-BLAST Web server: A remote homology search tool for relating protein domains. Nucl. Acids Res. 34, W143-W146.

* Pugalenthi, G., Shameer, K. Srinivasan, N. & Sowdhamini, R. (2006). HARMONY: a web-server for the assessment of protein structures Nucl. Acids Res. 34, W143-W146.

Pugalenthi, G. & Sowdhamini, R. (2006). iMOTdb - a comprehensive collection of spatially interacting motifs in proteins. Nucl. Acids Res. 34, D285-D286.

Ajay, S.M. & Bhalla, U.S. (2006). Synaptic plasticity in vitro and in silico: insights into an intracellular signaling maze. Physiology (Bethesda), 21, 289-296.

Bhaduri, A. & Sowdhamini, R. (2006). Domain architectural census of eukaryotic gene products containing O-protein phosphatases. Gene, 366, 246-255.

2005

Blaise, M., Sowdhamini,R. & Pradhan, N. (2005). Comparative analysis of different competitive antagonists interaction with NR2A and NR2B subunits of N-methyl-D-aspartate (NMDA) ionotropic glutamate receptor. J. Mol. Model. 11, 489-502.

Gaurav, K., Gupta, N. & Sowdhamini, R. (2005). FASSM: Enhanced Function Association in whole genome analysis using Sequence and Structural Motifs. In Silico Biol. 5, 425-438.

Le Novere, N., Finney, A., Hucka, M., Bhalla, U.S., Campagne, F., Collado-Vides, J., Crampin, E., Halstead, M., Klipp, E., Mendes, P., Nielsen, P., Sauro, H., Shapiro, B., Snoep, J. L., Spence, H. G. & Wanner, B.L. (2005). Minimal Information Requested In the Annotation of biochemical Models (MIRIAM). Nature Biotech. 23, 1509-1515.

Hayer, A. & Bhalla, U. S. (2005). Molecular Switches at the Synapse Emerge from Receptor and Kinase Traffic. PLoS Comput. Biol. 1, e20.

* Sandhya, S., Chakrabarti, S., Abhinandan, K.R., Sowdhamini, R. & Srinivasan, N. (2005). Assessment of a Rigorous Transitive Profile Based Search Method to Detect Remotely Similar Proteins. J. Biomol. Strc. Dyn. 23, 283-298.

Metpally, R.R. & Sowdhamini, R. (2005). Cross genome phylogenetic analysis of Human and Drosophila G-protein-coupled receptors: Application to functional annotation of orphan receptors. BMC Genomics, 6, 106.

Bhaduri, A. & Sowdhamini, R. (2005). Genome-wide survey of prokaryotic O-protein phosphatases. J. Mol. Biol. 352, 736-752.

Metpally, R.R. & Sowdhamini, R. (2005). Genome wide survey of G protein-coupled receptors in Tetraodon nigroviridis. BMC Evol. Biol. 5, 41.

Chakrabarti, S., Anand, A.P., Bhardwaj, N., Pugalenthi, G. & Sowdhamini, R. (2005). SCANMOT: searching for similar sequences using a simultaneous scan of multiple sequence motifs. Nucl. Acids Res. 33, W274-W276.

Pugalenthi, G., Archunan, G. & Sowdhamini, R. (2005). DIAL: a web-based server for the automatic identification of structural domains in proteins. Nucl. Acids Res. 33, W130-W132.

Pugalenthi, G., Bhaduri, A. & Sowdhamini, R. (2005). GenDiS: Genomic Distribution of Protein Structural Superfamilies. Nucl. Acids Res. 33, D252-D255.

Rajasethupathy, P., Vayttaden, S. J. & Bhalla, U. S. (2005). Systems modeling: a pathway to drug discovery. Curr. Opin. Chem. Biol. 9, 400-406.

HarshaRani, G. V., Vayttaden, S. J. & Bhalla, U. S. (2005). Electronic data sources for kinetic models of cell signaling. J. Biochem. 137, 653-657.

Thangudu, R.R., Vinayagam, A., Pugalenthi, G., Manonmani, A., Offmann, B. & Sowdhamini, R. (2005). Native and modelled disulphide bonds in proteins: Knowledge-based approaches towards structure prediction of disulphide-rich polypeptides Proteins Str. Fn. Bioinf. 58, 866-879.

Blaise, M.-C., Bhattacharyya, D., Sowdhamini, R. & Pradhan, N. (2005). Structural Consequences of D481N/K483Q Mutation at Glycine Binding Site of NMDA Ionotropic Glutamate Receptors: A Molecular Dynamics Study. J. Biomol. Struct. Dyn. 22, 399-410.

2004

Chakrabarti, S., Bhardwaj, N., Anand, P. & Sowdhamini, R. (2004). Improvement of alignment accuracy utilizing sequentially conserved motifs. BMC Bioinformatics, 5, 167.

Blaise M.C., Sowdhamini R., Metpally, R. P. R. & Pradhan N. (2004). Evolutionary Trace Analysis of Ionotropic Glutamate Receptors and Modeling the Interactions of Agonists with Different NMDA Receptor Subunits. J. Mol. Model. 10, 305-316.

Ajay, S. M. & Bhalla, U. S. (2004). A role for ERKII in synaptic pattern selectivity on the time-scale of minutes. Eur. J. Neurosci. 20, 2671-2680.

Sinha, D, Bhalla U. S. & Shivashankar, G. V. (2004). Kinetic measurement of ribosome motor stalling force. App. Phys. Lett. 85, 4789-4791.

Bhalla, U. S. (2004). Signaling in small subcellular volumes. I. Stochastic and diffusion effects on individual pathways. Biophys. J. 87, 733-744.

Bhalla, U. S. (2004). Signaling in small subcellular volumes. II. Stochastic and diffusion effects on synaptic network properties. Biophys. J. 87, 745-753.

Vasudeva, K, & Bhalla, U. S. (2004). Adaptive stochastic-deterministic chemical kinetic simulations. Bioinformatics, 20, 78-84.

Chakrabarti, S. & Sowdhamini, R. (2004). Regions of minimal structural variation among members of protein domain superfamilies: Application to remote homology detection and modelling using distant relationships. FEBS Lett. 569, 31-36.

Bhaduri, A., Pugalenthi, G. & Sowdhamini, R. (2004). PASS2: an automated database of protein alignments organised as structural superfamilies. BMC Bioinformatics, 5, 35.

Bhaduri, A., Pugalenthi, G., Gupta, N. & Sowdhamini, R. (2004). iMOT: an interactive package for the selection of spatially interacting motifs. Nucl. Acids Res. 32, W602-W605.

Innis, C.A., Anand, P.A. & Sowdhamini, R. (2004). Prediction of Functional Sites in Proteins using Conserved Functional Group Analysis. J. Mol. Biol. 337, 1053-1068.

Vinayagam, A., Pugalenthi, G., Rajesh, T. & Sowdhamini, R. (2004). DSDBASE: A consortium of native and modelled disulphide bonds in proteins. Nucl. Acids Res. 32, D200-D202.

Chakrabarti, S., John, J. & Sowdhamini, R. (2004). Improvement of comparative modeling by the application of conserved motifs amongst distantly related proteins as additional restraints. J. Mol. Model. 10, 69-75.

Bhaduri, A., Ravishankar, R. & Sowdhamini, R. (2004). Conserved spatially interacting motifs of protein superfamilies: Application to fold recognition and function annotation of genome data. Proteins, 54, 657-670.

Vayttaden, S. J., Ajay, S. M. & Bhalla, U. S. (2004). A spectrum of models of signaling pathways. ChemBioChem. 5, 1365-1374.

Bhalla, U. S. (2004). Models of cell signaling pathways. Curr. Opin. Genet. Dev. 14, 375-381.

Vayttaden, S. J. & Bhalla, U. S. (2004). Developing Complex Signaling Models using GENESIS/Kinetikit. Sci STKE. 219, 14.

2003

Bhalla, U. S. (2003). Temporal computation by synaptic signaling pathways. J. Chem. Neuroanat. 26, 81-86.

Bhalla, U. S. (2003). Managing models of signaling networks. Neurocomputing, 52-54, 215-220.

Sivakumaran, S., Hariharaputran, S., Mishra, J. & Bhalla, U. S. (2003). The Database of Quantitative Cellular Signaling: Repository and analysis tools for chemical kinetic models of signaling networks. Bioinformatics, 19, 408-415.

Bhalla, U. S. (2003). Understanding complex signaling networks through models and metaphors. Prog. Biophys. Mol. Biol. 81, 45-65.

Bhaduri, A. & Sowdhamini, R. (2003). A Genome-wide Survey of Human Tyrosine Phosphatases. Protein Eng. 16, 881-888.

* Sandhya, S., Kishore, S., Sowdhamini, R. & Srinivasan. N. (2003). Effective detection of remote homologues by searching in sequence dataset of a protein domain fold. FEBS Lett. 552, 225-230.

Vinayagam, A., Shi, J., Pugalenthi, G., Meenakshi, B., Blundell, T.L. & Sowdhamini, R. (2003). DDBASE2.0: Updated Domain Database with Improved Methods for the Identification of Structural Domains. Bioinformatics, 19, 1760-1764.

Chakrabarti,S., Venkataramanan, K. & Sowdhamini, R. (2003). SMoS: A database of Structural Motifs of Superfamilies. Protein Eng. 16, 791-793.

Chakrabarti, S. & Sowdhamini, R. (2003). Functional sites and evolutionary connections of Acyl Homoserine Lactone synthases. Protein Eng. 16, 271-278.

Bhaduri, A., Krishnaswamy, L., Ullal, G.R., Panicker, M.M. & Sowdhamini, R. (2003) Fold prediction and comparative modeling of Bdm1: a probable a/b hydrolase associated with hot water epilepsy. J. Mol. Model. 9, 3-8.

2002

Mishra, J. & Bhalla, U. S. (2002). Simulations of inositol phosphate metabolism and its interaction with InsP3 mediated calcium release. Biophys. J. 83, 1298-1316.

Bhalla, U. S., Ram, P. & Iyengar, R. (2002). MAP kinase phosphatase as a locus of flexibility in a mitogen-activated protein kinase signaling network. Science, 297, 1018-1023.

Bhalla, U. S. (2002). Mechanisms for temporal tuning and filtering by postsynaptic signaling pathways. Biophys. J. 83, 740-752.

Bhalla, U. S. (2002). Temporal pattern decoding by synaptic signaling pathways. J. Comput. Neurosci. 13, 49-62.

Bhalla, U. S. (2002). The chemical organization of signaling interactions. Bioinformatics, 18, 855-863.

Bhalla, U. S. (2002). Use of Kinetikit and GENESIS for modeling signaling pathways. Methods Enzymol. 345, 3-23.

Bhaduri, A., Mallika, V. & Sowdhamini, R. (2002). Genome Analysis of PASS2 a Semi Automated Database of Protein Alignments Organised as Structural Superfamilies. Sci. World J., 2, 9-10.

Mallika, V., Bhaduri, A. & Sowdhamini, R. (2002). PASS2: A semi-automated database of protein alignments organised as structural superfamilies. Nucl. Acids Res. 30, 284-280.

* Pandit, S.B., Gosar, D., Abhiman, S., Sujatha, S., Dixit, S.B., Mhatre, N.S., Sowdhamini, R. & Srinivasan, N. (2002). SUPFAM -Database of potential protein superfamily relationships derived by comparing sequence-based and structure-based families: Implications for structural genomics and function annotation in genomes. Nucl. Acids Res. 30, 289-293.

NATIONAL CHEMICAL LABORATORY, PUNE.

2006

Jitendra, G. & Vishwas, C. (2006). Open access and biodiversity conservation: Changes and potentials for the developing world. Data Science Journal, 5, 1-17.

Chavan, V. & Aniruddha, K. (2006). Open Access geospatial data repository. Curr. Sci. 90, 617-618.

2005

Vishwas, C., Achuthankutty, C.T., Edward, V. B. & Mohideen, W. (2005). Indobis an Ocean Biogeographic Information System for assessment and conservation of Indian Ocean biodiversity. Indian Journal of Marine Sciences, 34, 120-127.

Vishwas, C., Nilesh, R., Aparna, W. & Michael, R. (2005). Resolving Taxonomic Discrepancies : Role of Electronic Catalogues of Known Organisms. Journal Biodiversity Informatics, 2, 70-78.

Chavan, V., Rane, N. S., Ghate, H. V. & Krishnan, S. (2005). IndCollections: biological specimens in Indian collections. Curr. Sci. 89, 1454-1455.

2004

Chavan, V., Watve, A. V., Londhe, M. S., Rane, N. S., Pandit, A. T. & Krishnan, S. (2004). Cataloguing Indian biota: the electronic catalogue of known Indian fauna. Curr. Sci, 87, 749-763.

Watve, A. V., Gaikwad, J. & Vishwas, C. (2004). Accessing biological collections data of Indian origin. Curr. Sci. 86, 8.

2003

Chavan, V., Watve, A. V. & Krishnan, S. (2003). Electronic catalogue of known Indian fauna. Curr. Sci. 85, 1515.

Chavan, V. & Krishnan, S. (2003). Natural history collections: a call for national information infrastructure. Curr. Sci. 84, 34-42.

NATIONAL DAIRY RESEARCH INSTITUTE, Karnal.
2007

Yadav, A., Yadav, B. R. & Mandhan, R. P. (2007). Genetic diversity among six breeds of Indian goat using RAPD markers. Biotechnol. 6, 57–60.

2006

De, S. & Singh, R. K. (2006). Identification of new MHC-DRB3 alleles from Indian (Bos indicus) cattle. Anim. Genet. 37, 605.

Mukherjee, S. & Yadav, B. R. (2006). Differential banding patterns in sex chromosomes of crossbred goats. Indian J. Dairy Sci. 59, 252–256.

Sharma, A. K., Sharma, R. K. & Kasana, H. S. (2006). Empirical comparisons of feed-forward connectionist and conventional regression models for prediction of first lactation 305-day milk yield in Karan Fries dairy cows. Neural Comput. Appl. 15, 359–365.

Sharma, A. K., Sharma, R. K. & Kasana, H. S. (2006). Prediction of first lactation 305-day milk yield in Karan Fries dairy cattle using ANN modeling. Appl. Soft Comput. 7, 1112-1120.

Yadav, A., Yadav, B. R. & Mandhan, R. P. (2006). Sex chromosome polymorphisms in three breeds of goats. J. Cytol. Genet. 7, 39–42.

2005

Jain, D. K., Sharma, A. K. & Ruhil, A. P. (2005). Role of information technology in dairy science: a review. Indian J. Anim. Sci. 75, 985–991.

Jiang, Z., De, S., Gracia, M. D., Griffin, K. B., Wu, X. L., Xiao, Q., Michal, J. J., Sharma, B. S. & Jansen, G. B. (2005). An independent confirmation of a quantitative trait locus for milk yield and composition traits on bovine chromosome 26. J. Anim. Breed. Genet. 122, 281–284.

Wu, X.L., MacNeil, M. D., De, S., Xiao, Q. J., Michal, J. J., Gaskins, C. T., Reeves, J. J., Busboom, J. R., Wright Jr., R. W. & Jiang, Z. (2005). Evaluation of candidate gene effects for beef back fat via Bayesian model selection. Genetica, 125, 103–113.

2004

Ganguly, I., Sarma, A., De, S. & Mitra, A. (2004). Genetic polymorphism of BoLA-DRB3.2 locus in crossbred cattle as revealed by PCR-RFLP analysis. Indian J. Anim. Sci. 74, 195–199.

Parmar, S. N. S., Yadav, B. R. & Srivastava, P. N. (2004). Genetic diversity between Malvi and Nimari breeds of Zebu cattle using RAPD markers. Indian J. Anim. Sci. 74, 281–284.

Shende, P. K. & Yadav, B. R. (2004). Genetic diversity analysis in Nagpuri vis-à-vis Murrah buffalo using randomly amplified polymorphic DNA markers. Buffalo J. 20, 161–172.

2002

De, S., Singh, R. K. & Buchaiah, G. (2002). MHC-DRB exon 2 allele polymorphism in Indian River buffalo (Bubalus bubalis). Anim. Genet. 33, 215–219.

NATIONAL INSTITUTE OF IMMUNOLOGY, NEW DELHI.

2007

Kumar, N. & Mohanty, D. (2007). MODPROPEP: A program for knowledge based modeling of protein-peptide complexes. Nucl. Acids Res. (In press).

Goyal, K., Mohanty, D. & Mande, S. C. (2007). PAR-3D: A server to predict protein active site residues. Nucl. Acids Res. (In press).

Hansia, P., Dev, S., Surolia, A. & Vishveshwara, S. (2007). Insight into the early stages of thermal unfolding of peanut agglutinin by molecular dynamics simulations. Proteins Str. Fn. Bioinf. (In press).

2006

Krithika, R., Marathe, U., Saxena, P., Ansari, M. Z., Mohanty, D. & Gokhale, R. S. (2006). A genetic locus required for iron acquisition in Mycobacterium tuberculosis. Proc. Natl. Acad. Sci. USA, 103, 2069-2074.

Sethi, D. K., Agarwal, A., Manivel V, Rao K. V. S. & Salunke D. M. (2006). Differential epitope positioning within the germline antibody paratope enhances promiscuity in the primary immune response. Immunity. 24, 429-438.

2005

Trivedi, O. A., Arora, P., Vats, A., Ansari, M. Z., Tickoo, R., Sridharan, V., Mohanty, D. & Gokhale, R. S. (2005). Dissecting the mechanism and assembly of a complex virulence mycobacterial lipid. Mol. Cell, 17, 631-643.

Kamra, P., Gokhale, R. S. & Mohanty, D. (2005). SEARCHGTr: a program for analysis of glycosyltransferases involved in glycosylation of secondary metabolites. Nucl. Acids Res. 33, W220-W225.

2004

Ansari, M. Z., Yadav, G., Gokhale, R. S. & Mohanty, D. (2004). NRPS-PKS: a knowledge-based resource for analysis of NRPS/PKS megasynthases. Nucl. Acids Res. 32, W405-W413.

Trivedi, O. A., Arora, P., Sridharan, V., Tickoo, R., Mohanty, D. & Gokhale, R. S. (2004). Enzymic activation and transfer of fatty acids as acyl-adenylates in mycobacteria. Nature, 428, 441-445.

Sudha, R., Anantharaman, L., Sivaram, M.V., Mirsamadi, N., Choudhury, D., Lohiya, N. K., Gupta, R. B. & Roy, R. P. (2004). Linkage of interactions in sickle hemoglobin fiber assembly: inhibitory effect emanating from mutations in the AB region of the alpha-chain is annulled by a mutation at its EF corner. J. Biol. Chem. 279, 20018-20027.

2003

Yadav, G., Gokhale, R. S. & Mohanty, D. (2003). Computational approach for prediction of domain organization and substrate specificity of modular polyketide synthases. J. Mol. Biol. 328, 335-363.

Yadav, G., Gokhale, R. S. & Mohanty, D. (2003). SEARCHPKS: A program for detection and analysis of polyketide synthase domains. Nucl. Acids Res. 31, 3654-3658.

Saxena, P., Yadav, G., Mohanty, D., Gokhale, R.S. (2003). A new family of type III polyketide synthases in Mycobacterium tuberculosis. J. Biol. Chem. 278, 44780-44790.

Nair, D. T., Kaur, K. J., Singh, K., Mukherjee, P., Rajagopal, D., George, A., Bal, V., Rath, S., Rao, K. V. S. & Salunke, D. M. (2003). Mimicry of native peptide antigens by the corresponding retro-inverso analogs is dependent on their intrinsic structure and interaction propensities. J. Immunol. 170, 1362-1373.

2002

Nagpal, S., Kaur, K. J., Jain, D. & Salunke, D. M. (2002). Plasticity in structure and interactions is critical for the action of indolicidin, an antibacterial peptide of innate immune origin. Protein Sci. 11, 2158-2167.

Nair, D. T., Singh, K., Siddiqui, Z., Nayak, B. P., Rao, K. V. S. & Salunke, D. M. (2002). Epitope Recognition by diverse antibodies suggests conformational convergence n an antibody response. J Immunol. 168, 2371-2382.

PANJAB UNIVERSITY, CHANDIGARH.

2007

Nandel, F. S. & Saini, A. (2007). Conformational Study of Short Peptoid Models for Future Applications as Potent Antimicrobial Compounds. Macromolecular Theory and Simulations, 16, 295-303.

Nandel, F. S. & Saini, A. (2007). Construction and design of single stranded collagen-like structure. Indian Journal of Biochemistry & Biophysics, 44, 106-113.

2005

Nandel, F. S. & Khare, B. (2005). Conformation of peptides Constructed from Achiral Amino Acid Residues Aib and DZPhe: Computational study of the Effect of L/D- Leu at terminal positions. Biopolymers, 77, 63-73.

2003

Nandel, F. S. & Harpreet, K. (2003). Effect of terminal achiral and chiral residues on the conformational behaviour of poly Dz Phe and analysis of various interactions. Indian J. Biochem & Biophysics, 40, 265-273.

PONDICHERRY UNIVERSITY, PONDICHERRY.

2006

Shanthi, N. & Parthiban, M. (2006). Binding site prediction of galanin peptide using evolutionary trace method. Bioinformation, 1, 180-183.

Tresha, R. A. T. & Shanthi, N. (2006). DrugMetZ DB: an anthology of human drug metabolizing enzymes. Bioinformation, 1, 248–250.

2005

Sundar, D., K. Kandavelou, M. Mani, Wu, J., Porteus, M.H. & Chandrasegaran, S. (2005). Zinc finger nucleases: custom-designed molecular scissors for genome engineering of plant and mammalian cells. Nucl. Acids Res. 33, 5978-5990.

2004

Swarnalatha, M., Jutur, P.P., Amouda, V., Mathur, P.P. & Reddy, A.R. (2004). Prediction of Transcriptional Regulation by Dlx and Msx homeodomain proteins. Online J. Bioinformatics, 5, 132-145.

Mathur, P.P. (2004). Bioinformatics: From Pre-Genomic to Post-Genomic Era. *Adv. Biotech.* 3, 27-31.

RAJIV GANDHI CENTRE FOR BIOTECHNOLOGY, THIRUVANANTHAPURAM.

2007

Hariharan, R. & Pillai, M. R. (2007). Structure-function relationship of Inhibitory Smads: Structural flexibility contributes to functional divergence. *BMC Struct. Biol.* (In press).

2006

Hariharan, R. & Pillai, M. R. (2006). Homology modeling of the DNA-binding domain of human Smad5: A molecular model for inhibitor design. *J. Mol. Graph. Mod.* 24, 271-277.

Joy, S., Nair, P. S., Hariharan, R. & Pillai, M. R (2006). Detailed comparison of the protein-ligand docking efficiencies of gold, a commercial package and Arguslab, a licensable freeware. *In Silico Biol.* 6, 601-605.

SAHA INSTITUTE OF NUCLEAR PHYSICS, KOLKATA.

2007

* The NMITLI-BioSuite Team (2007) BioSuite: A comprehensive bioinformatics software package (A unique industry academia collaboration). *Curr. Sci.* 92, 29-38.

Varadwaj, P. R. (2007). Quantum chemical investigation of linear hydrogen bonding in ONCCN center dot center dot center dot HX (X = F, Cl, Br) dimers, *Int. J. Quant. Chem.* 107, 1194-1204.

2006

* Mukherjee, S., Bansal, M. & Bhattacharyya, D. (2006). Conformational specificity of non-canonical base pairs 4 and higher order structures in nucleic acids: crystal 5 structure database analysis. *J. Comp. Aided Mol. Des.* 20, 629-645.

Das, J., Mukherjee, S., Mitra, A. & Bhattacharyya, D. (2006). Non-Canonical Base Pairs and Higher Order Structures in Nucleic Acids: Crystal Structure Database Analysis. *J. Biomol. Struct. Dyn.* 24, 149-161.

Bandyopadhyay, D. & Bhattacharyya, D. (2006). Estimation of Strength in different Extra Watson-Crick Hydrogen Bonds in DNA Double Helices through Quantum Chemical studies. *Biopolymers*, 83, 313-325.

Sen, K., Basu, S. & Bhattacharyya, D. (2006). Ab Initio Studies on Excited State Intramolecular Electron Transfer in 4-Amino-N-Methylphthalimide and 3- Amino-N-Methylphthalimide. *Int. J. Quant. Chem.* 106, 913-927.

Banerjee, A. & Sengupta, P. K. (2006). Encapsulation of 3-hydroxyflavone and fisetin in beta-cyclodextrins: Excited state proton transfer fluorescence and molecular mechanics studies, Chem. Phys. Lett. 424, 379-386.

Banerjee, A., Sengupta, B., Chaudhuri, S., Basu, K. & Sengupta, P. K. (2006). Encapsulation of Prodan in beta-cyclodextrin environments: A critical study via electronic spectroscopy and molecular mechanics. J. Mol. Struct. 794, 181-189.

Varadwaj, P. R. & Jaman, A. I. (2006). Centrifugal distortion analysis of the millimeter-wave spectrum of 2- fluorobenzonitrile and ab initio DFT calculations. J. Mol. Spectrosc. 236, 70-74.

Varadwaj, P. R. & Jaman, A. I. (2006). Millimeter-wave spectrum of 2, 3-difluorobenzonitrile and ab initio DFT calculations. J. Mol. Spectrosc. 239, 216-220.

Bhattacharyya, M., Mukhopadhyay, C. & Chakrabarti, A. (2006). Specificity of prodan for the self-associating domain of spectrin: A Molecular docking study J. Biomol. Struct. Dyn. 24, 269-276.

2005

Blaise, M. C., Bhattacharyya, D., Sowdhamini, R. & Pradan, N. (2005). Structural consequences of D481N/K483Q mutation at glycine binding site of NMDA ionotropic glutamate receptors: a molecular dynamics study. J. Biomol. Struct. Dyn. 22, 399-410.

Bhattacharyya, D., Sen, K. & Mukherjee, S. (2005). Non-planar Amino Groups: Protein Structure Database Analysis and Ab Initio Quantum Chemical Studies on Model Systems, Ind. J. Chem. A (Special Issue on Chemoinformatics and Computer Aided Drug Design) 45A, 58-67.

Mukherjee, S., Majumdar, S. & Bhattacharyya, D. (2005). Role of Hydrogen Bonds in Protein-DNA Recognition: Effect of Non-planar Amino Groups. J. Phys. Chem. B, 109, 10484-10492.

* Basu, S., Majumdar, R., Das, G.K. & Bhattacharyya, D. (2005). Energy Barriers and Rates of Tautomeric Transitions in DNA Bases: Ab initio Quantum Chemical Study, Ind. J. Biochem. Biophys. 42, 378-385.

Bakshi, K. & Bhattacharya, N. P. (2005). Substitution of polymorphic amino acids in proteins: Predicting functional alterations using amino acid properties. Online J. Bioinf. 6, 42-50.

2004

Mukherjee, S. & Bhattacharyya, D. (2004). Effect of Phosphorothioate Chirality on the Grooves of DNA Double Helices: A Molecular Dynamics Study. Biopolymers, 73, 269-282.

* Dasgupta, A. K., Majumdar, R. & Bhattacharyya, D. (2004). Characterization of non-planar peptide groups in protein crystal structures. Ind. J. Biochem. Biophys. 42, 49-55.

Sen, K., Basu, S. & Bhattacharyya, D. (2004). QM/MM study of excited state electron transfer between pyrene and 4,4-Bis (dimethylamino) diphenylmethane with different solvent systems: role of hydrogen bonding within solvent molecules. Inter. J. Quant. Chem. 102, 368-378.

Sengupta, B., Banerjee, A. & Sengupta, P. K. (2004). Investigations on the binding and antioxidant properties of the plant flavonoid fisetin in model biomembranes. FEBS Lett. 77, 77-81.

Sampa, B. (2004). Functional properties of Soybean Nodulin26 from a comparative three dimensional model. FEBS Lett. 558, 39-44.

Sen, U., Dasgupta, J., Choudhury, D., Datta, P., Chakrabarti, A., Chakrabarty, S. B., Chakrabarty, A. & Dattagupta, J. K. (2004). Crystal structures of HbA2 and HbE and modeling of Hemoglobin d4: interpretations of the thermal stability and the antisickling effect of HbA2. Biochemistry, 43, 12477-12488.

2003

Maji, S. K., Haldar, D., Bhattacharyya, D. & Banerjee, A. (2003). Conformational heterogeneity of a turn mimetic pseudo-peptide: comparison of crystal state, solution and theoretically derived structures, J. Mol. Struct. 646, 111-123.

Bandyopadhyay, D. & Bhattacharyya, D. (2003). Different Modes of Interaction between hydrated magnesium ion and DNA functional groups: Database analysis and ab initio studies. J. Biomol. Struct. Dyn. 21, 447-458.

Banerjee, R., Sen, M., Bhattacharya, D. & Saha, P. (2003). The Jigsaw Puzzle Model: Search for Conformational Specificity in Protein Interiors. J. Mol. Biol. 333, 211-226.

Dasgupta, J., Sen, U. & Dattagupta, J. K. (2003). In silico mutations and molecular dynamics studies on a winged bean chymotrypsin inhibitor protein. Protein Eng. 16, 489-496.

2002

Bandyopadhyay, D. & Bhattacharyya, D. (2002). Effect of flanking residues on CA and AA dinucleotides: Some rationale. J. Biomol. Struct. Dyn. 19, 659-667.

TEZPUR UNIVERSITY, ASSAM.

2006

Das, D., Satapathy, S. S., Buragohain, A. K. & Ray, S. K. (2006). Occurrence of all nucleotide combinations at the third and the first positions of two adjacent codons in open reading frames of bacteria. Curr. Sci. 90, 22-24.

2005

Verma, S. K., Das, D., Satapathy, S. S., Buragohain, A. K. & Ray, S.K. (2005). Compositional Symmetry of DNA Duplex in Bacterial Genomes. Curr. Sci. 89, 374-384.

Das, D., Verma, S. K. & Ray, S. K. (2005). An Altered G + C% Region Within Potential Hemagglutinin ORFs of Ralstonia solanacearum. Curr. Sci. 88, 786-792.

UNIVERSITY INSTITUTE OF CHEMICAL TECHNOLOGY, MUMBAI.

2007

Vepuri, S. B., Tawari, N. & Degani, M. S. (2007). Quantitative Structure Activity Relationship Study of Some Aspartic Acid Analogues to Correlate and Predict their Sweetness Potency. QSAR & Combinatorial Science, 26, 204-214.

Subbihya, R., Bag, S., Tawari, N. & Degani, M. S. (2007). 3D-QSAR Analysis of 2-(oxalylamino) benzoic acid class of Protein Tyrosine Phosphatase 1B Inhibitors by CoMFA and Cerius2.GA. QSAR & Combinatorial Science, 26, 608-617.

2004

Kelkar, M. A., Pednekar D. V., Pimple, S. R. & Akamanchi, K. G. (2004). 3D QSAR Studies of Inhibitors of Cholesterol Ester Transfer Protein (CETP) by CoMFA, CoMSIA and GFA Methodologies. Med. Chem. Res. 8, 590-604.

Pednekar, D. V., Kelkar, M. A., Pimple, S. R. & Akamanchi, K. G. (2004). 3D QSAR Studies of Inhibitors of Epidermal Growth Factor Receptor [EGFR] Using CoMFA and GFA Methodologies. Med. Chem. Res. 8, 604-618.

Pimple, S. R., Kelkar, M. A., Pednekar D. V. & Akamanchi, K. G. (2004). Studies On Novel Non-Imidazole Human H4 Receptor Antagonists Using GFA And Free-Wilson Analysis. Med. Chem. Res. 8, 619-630.

UNIVERSITY OF AGRICULTURE, MANGALORE.

2007

* Malathi, S., Karunasagar, I. & Karunasagar, I. (2007). Abundance, composition and distribution of simple sequence repeats and dinucleotide compositional bias within WSSV genomes. Ind. J. Genet. (In press).

* Rekha, K., Malathi, S., Indrani, K. & Karunasagar, I. (2007). A bioinformatic based study of OmpTS protein of Aeromonas hydrophila : a potential vaccine candidate for aquaculture. Aquaculture (In press).

2006

* Godhe, A., McQuoid, M.R., Karunasagar, I., Karunasagar, I. & Rehnstam Holm Ann S. (2006). Comparison of three common molecular tools for distinguishing among geographically separated clones of the diatom Skeletonema marinoi sarno et zingone (Bacillariophyceae). J. Phycol. 42, 280-291.

Parvathi, A., Sanath, K. H., Karunasagar, I. & Karunasagar,I. (2005). Study of occurrence of V.vulnificus by RAPD and gyrB sequence analysis. Environ. Microbiol. 7, 995-1002.

* Malathi, S., Karunasagar, I. & Karunasagar, I. (2005). A computer based identification of variable number of tandem repeats in White Spot Syndrome Virus (WSSV) genomes. Curr. Sci. 89, 882-887.

Manjanaik, B., Umesha, K.R., Karunasagar, I. & Karunasagar, I. (2005). Detection of hepatopancreatic parvovirus (HPV) in wild shrimps in India by nested polymerase chain reaction (PCR). DAO. 63, 255-259.

2004

Shahadat, H. Md., Otta, S. K., Chakraborty, A., Sanath, K.H., Karunasagar, I. & Karunasagar, I. (2004). Detection of WSSV in cultured shrimps, captured brooders, shrimp postlarvae and water samples in Bangladesh by PCR using different primers. Aquaculture, 237, 59-71.

Manivannan, S., Bob, K.M.D., Karunasagar, I. & Karunasagar, I. (2004). Prevalence of monodon baculovirus (MBV) in wild Metapenaeus species along the south west coast of India. Aquaculture, 232, 63-67.

2003

* Dhanashree, B., Otta, S.K., Karunasagar, I., Goebel, W. & Karunasagar, I. (2003). Incidence of Listeria spp. in clinical and food samples in Mangalore, India. Food Microbiol. 20, 447-453.

* Dhanashree, B., Otta, S.K., Karunasagar, I. & Karunasagar, I. (2003). Protein profile analysis of Listeria monocytogenes strains from tropics. Curr. Sci. 84, 628-630.

Karunasagar, I., Rivera, B., Joseph, B., Kennedy, V.R., Shetty, A., Huq, I., Karunasagar, I. & Colwell R.R. (2003). OmpU genes in nontoxigenic V.cholerae associated with aquaculture. J. Appl. Microbiol. 95, 338-343.

2002

* Chakraborty, A., Otta, S.K., Joseph, B., Sanath, K.H., Shahadat, H. Md.., Karunasagar I., Venugopal, M.N. & Karunasagar I. (2002). Prevalence of white spot syndrome virus (WSSV) in wild crustaceans along the coast of India. Curr. Sci. 82, 1392-1397.

* Manivannan, S., Otta, S.K., Karunasagar, I. & Karunasagar, I. (2002). Multiple viral infection in Penaeus monodon shrimp postlarvae in an Indian hatchery. DAO. 48, 233-236.

UNIVERSITY OF ALLAHABAD, ALLAHABAD.

2007

Srinivasan, N. (2007). Cognitive Neuroscience of Creativity: EEG based Approaches. Methods, 42, 109-116

Dietrich, A., & Srinivasan, N. (2007). The optimal age to start a revolution. J. Creative Behavior (In press).

2006

Srinivasan, N. & Brown, J. M. (2006). Effects of endogenous visual attention on the detection and discrimination of spatial frequencies. Perception, 35, 193-200.

Rimzhim, Sunny, M. M. & Srinivasan, N. (2006). Cerebral Hemispheric Asymmetry in Semantic Categorization: Does the Nature of Stimulus matter? Annals. Neurosci. (Suppl.), 13, 45.

2004

Essock, E. A., Sinai, M. J., DeFord, J. K., Hansen, B. & Srinivasan, N. (2004). Human perceptual performance with nighttime imagery: Region recognition and texture-based segmentation. J. Exp. Psychol. Appl. 10, 97-110.

2003

Dutt, D. N., Krishnan, S. M. & Srinivasan, N. (2003). A dynamic nonlinear time domain model for reconstruction and compression of cardiovascular signals with application to telemedicine. Comput. Biol. Med. 33, 45-63.

Ravichandran, V. & Srinivasan, N. (2003). Stable states and sufficient conditions for correct retrieval in the bidirectional associative memory. IETE J. Res. 49, 55-58.

UNIVERSITY OF CALCUTTA, KOLKATA.

2005

* Basu, S., Majumdar, R., Das, G. K. & Bhattacharyya, D. (2005). Energy barriers and rates of tautomeric transitions in DNA bases: ab initio quantum chemical study. Indian J. Biochem. Biophys. 42, 378-385.

2004

* Dasgupta, A. K., Majumdar, R. & Bhattacharyya, D. (2004). Characterization of non-planar peptide groups in protein crystal structures. Indian J. Biochem. Biophys. 41, 233-240.

UNIVERSITY OF DELHI, NEW DELHI.

2007

Jain, M., Nijhawan, A., Arora, R., Agarwal, P., Ray, S., Sharma, P., Kapoor, S., Tyagi, A. K. & Khurana, J. P. (2007). F-box proteins in rice, Genome-wide analysis, classification, temporal and spatial gene expression during panicle and seed development, and regulation by light and abiotic stress. Plant Physiol. 143, 1467-1483.

The Rice Annotation Project. (2007). Curated genome annotation of Oryza sativa ssp. japonica and comparative genome analysis with Arabidopsis thaliana. Genome Res. 17, 175-183

Ravi, V., Khurana, J. P., Tyagi, A. K. & Khurana, P. (2007). Rosales sister to Fabales: towards resolving the rosid puzzle. Mol. Phylogenet. Evol. 44, 488-493.

* Singh, S., Samal, A., Giri, V., Krishna, S., Raghuram, N. & Jain, S. (2007). A Universal power law and proportionate change process characterizes the evolution of metabolic networks. Euro. Phys. J. B, 57,75-80.

2006

Jain, M., Kaur, N., Garg, R., Thakur, J. K., Tyagi, A. K. & Khurana, J. P. (2006). Structure and expression analysis of early auxin-responsive Aux/IAA gene family in rice (Oryza sativa). Funct. Integr. Genomics, 6, 47-59.

Jain, M., Kaur, N., Tyagi, A. K. & Khurana, J. P. (2006). Comprehensive analysis of auxin responsive GH3 gene family in rice (Oryza sativa). Funct. Integr. Genomics, 6, 36-46.

Jain, M., Tyagi, A. K. & Khurana, J. P. (2006). Molecular characterization and differential expression of cytokinin-responsive type-A response regulators in rice (Oryza sativa). BMC Plant Biol. 6, 1.

Jain, M., Tyagi, A. K. & Khurana, J. P. (2006). Overexpression of putative topoisomerase 6 genes from rice confers stress tolerance in transgenic Arabidopsis plants. FEBS J. 273, 5245-5260.

Jain, M., Tyagi, A. K. & Khurana, J. P. (2006). Genome-wide analysis, evolutionary expansion, and expression of early auxin-responsive SAUR gene family of rice (Oryza sativa). Genomics, 88, 360-371.

Kumar, M., Kulwal, P. L., Gaur, A., Tyagi, A. K., Khurana, J. P., Khurana, P., Balyan, H. S. & Gupta, P. K. (2006). QTL analysis for grain weight in common wheat. Euphytica, 151, 135-144.

Ravi, V., Khurana, J. P., Tyagi, A. K. & Khurana, P. (2006). The chloroplast genome of mulberry: complete nucleotide sequence, gene organization and comparative analysis. Tree Genet. Genomes, 3, 49-59.

Varshney, R. K., Hoisington, D. A. & Tyagi, A. K. (2006). Advances in cereal genomics and applications in crop breeding. Trends Biotechnol. 24, 490-497.

Vij, S., Gupta, V., Kumar, D., Vydianathan, R., Raghuvanshi, S., Khurana, P., Khurana, J. P. & Tyagi, A. K. (2006). Decoding the rice genome. Bioessays, 28, 421-432.

Vij, S. & Tyagi, A. K. (2006). Genome-wide analysis of the stress associated protein (SAP) gene family containing A20/AN1 zinc-finger(s) in rice and their phylogenetic relationship with Arabidopsis. Mol. Genet. Genomics, 276, 565-575.

* Samal, A., Singh, S., Giri, V., Krishna, S., Raghuram, N. & Jain, S.(2006). Low Degree metabolites explain essential reactions and enhance modularity in biological networks. BMC Bioinformatics, 7, 118.

2005

International Rice Genome Sequencing Project. (2005). The map-based sequence of the rice genome. Nature, 436, 793-800.

Kulshreshtha, R., Kumar, N., Balyan, H. S., Gupta, P. K., Khurana, P., Tyagi, A. K. & Khurana, J. P. (2005). Structural characterization, expression analysis and evolution of the red/far-red sensing photoreceptor gene, PHYTOCHROME C (PHYC) localized on the 'B' genome of hexaploid wheat (Triticum aestivum L.). Planta, 221, 675-689.

Kulwal, P., Kumar, N., Gaur, A., Khurana, P., Khurana, J. P., Tyagi, A. K., Balyan, H. S. & Gupta, P. K. (2005). Mapping of a major QTL for pre-harvest sprouting tolerance on chromosome 3A in bread wheat. Theor. Appl. Genet. 111, 1052-1059.

Mueller, L. A., Tanksley, S. D., Giovannoni, J. J., van, Eck, J., Stack, S., Choi, D., Kim, B. D., Chen, M., Cheng, Z., Li, C., Ling, H., Xue, Y., Seymour, G., Bishop, G., Bryan, G., Sharma, R., Khurana, J., Tyagi, A. K., Chattopadhyay, D., Singh, N., Stiekema, W., Lindhout, P., Jesse, T., Lankhorst, R. K., Bouzayen, M., Shibata, D., Tabata, S., Granell, A., Botella, M. A., Giuliano, G., Frusciante, L., Causse, M. & Zamir, D. (2005). The tomato sequencing project, the first cornerstone of the international Solanaceae project (SOL). Comp. Funct. Genom. 6, 153-158.

The Rice Chromosomes 11 and 12 Sequencing Consortia. (2005). The sequence of rice chromosomes 11 and 12, rich in disease resistance genes and recent gene duplication. BMC Biol. 3, 20.

2004

Singh, N. K., Raguvanshi, S., Srivastava, S. K., Gaur, A., Pal, A. K., Dalai, V., Singh, A., Ghazi, I. A., Yadav, M., Dixit, A., Batra, K., Gaikwad, K., Sharma, T. R., Mohapatra, T., Mohanty, A., Bharti, A. K., Kapur, A., Gupta, V., Kumar, D., Vij, S., Ravi, V., Khurana, P., Sharma, S., McCombie, D., Messing, J., Wing, R., Sasaki, T., Khurana, P., Khurana, J. P. & Tyagi, A. K. (2004). Sequence analysis of the long arm of rice chromosome 11 for rice-wheat synteny. Funct. Integr. Genomics, 4, 102-117.

2003

Thakur, J. K., Malik, M. R., Bhatt, V., Reddy, M. K., Sopory, S. K., Tyagi, A. K. & Khurana, J. P. (2003). A polycomb group gene of rice (Oryza sativa L. subsp. Indica), OsiEZ1, codes for a nuclear-localized protein expressed preferentially in young seedlings and during reproductive development. Gene, 314, 1-13.

2002

Chen, C., Presting, G., Barbazuk, W. B., Goicoehea, J. L., Blackmon, B., Fang, G., Kim, H., Frisch, D., Yu. Y., Higingbottom, S., Phimphilai, J., Phimphilai, D., Thurmond, S., Gaudette, B., Li., P., Lin, J., Hartfield, J., Main, D., Sun, S., Farrar, K., Henderson, C., Barnett, L., Costa, R., Williams, B., Walser, S., Atkins, M., Hall, C., Bancroft, I., Salse, J., Regad, F., Mohpatra, T., Singh, N. K., Tyagi, A. K., Soderlund, C., Dean, R. A. & Wing, R. A. (2002). An integrated physical and genetic map of the rice genome. Plant Cell, 14, 537-545.

UNIVERSITY OF HYDERABAD, HYDERABAD.

2007

Hemalatha, G. R., Rao, D. S. & Guruprasad, L. (2007). Identification and Analysis of Novel Amino-Acid Sequence Repeats in Bacillus anthracis str. Ames Proteome Using Computational Tools. Comp. Funct. Genomics. (In Press)

Annamala, M. K., Inampudi, K. K. & Guruprasad, L. (2007). Docking of phosphonate and trehalose analog inhibitors into M. tuberculosis mycolyltransferase Ag85C: Comparison of the two scoring fitness functions GoldScore and ChemScore, in the GOLD software. Bioinformation, 1, 339-350.

2006

Hemalatha, G. R., Swathi, A. & Guruprasad, L. (2006). Analysis and modeling of mycolyl-transferases in the CMN group. Bioinformation, 1, 161-169.

Hemalatha, G. R., Swathi, A. & Guruprasad, L. (2006). The Rv3799.Rv3807 gene cluster in Mycobacterium tuberculosis genome corresponds to the ancient conserved region in CMN mycolyltransferases. Evol. Bioinfo. Online, 2, 117-125.

Guruprasad, K., Kartik, V. J., Lavanya, T. & Guruprasad, L. (2006). Juxtaposed half-cystines as disulphide bridged partners in protein tertiary structure. Prot. Pept. Lett. 13, 577-579.

Nagini, M., Reddy, G. V., Hemalatha, G. R., Guruprasad, L. & Reddanna, P. (2006). Functional correlation of cyclooxygenases- 1, 2 and 3 from amino acid sequences and three dimensional model structures. Ind. J. Chem. 45A, 182-187.

2004

* Anindla, S., Inampudi, K.K., Guruprasad, K. & Guruprasad. L. (2004). Identification and analysis of novel tandem repeats in the cell surface proteins of Archaealand Bacterial genomes using computational tools. Comp. Funct. Genomics, 5, 2-16.

* Adindla, S., Guruprasad, K. & Guruprasad, L. (2004). Three-dimensional models and structure analysis of corynemycolyltransferases in Corynebacterium glutamicum and Corynebacterium efficiens. Int J Biol Macromol. 34, 181-189.

2003

* Guruprasad, K., Rao, M. J., Adindla, S. & Guruprasad. L. (2003). Combinations of turns in proteins. J. Pept. Res. 62, 167-174.

Adindla, S. & Guruprasad, L. (2003). Sequence analysis corresponding to the PPE and PE proteins in Mycobacterium tuberculosis and other genomes. J. Biosci. 28, 169-179.

* Guruprasad, K., Shukla, S., Adindla, S. & Guruprasad, L. (2003). Prediction of gamma-turns from amino acid sequences. J. Pept. Res. 61, 243-251.

UNIVERSITY OF KALYANI, WEST BENGAL.

2006

* Bagchi, A. & Ghosh, T. C. (2006). Structural study of two proteins SigE and ORF1 to predict their roles in the biochemical oxidation of sulfur anions via the global sulfur oxidation operon (sox). Comput. Biol. Chem. 30, 227-332.

2005

* Bagchi, A. & Ghosh, T. C. (2005). A structural study towards the understanding of the interactions of SoxY, SoxZ, and SoxB, leading to the oxidation of sulfur anions via the novel global sulfur oxidizing (sox) operon. Biochem. Biophys. Res. Commun. 335, 609-615.

* Bagchi, A. Roy, D. & Roy, P. (2005). Homology modeling of a transcriptional regulator soxr of the lithotrophic sulfur oxidation (sox) operon IN α- PROTEOBACTERIA. J. Biomol. Struct. Dyn. 22, 571-578.

Bandyopadhyay, S., Bagchi, A. & Maulik, U. (2005) Active site driven ligand design: an evolutionary approach. J. Bioinfo. Comput. Biol. 3, 1053-1070.

UNIVERSITY OF PUNE, PUNE.

2007

* Greenbaum, J. A., Andersen, P. H., Blythe, M., Bui, H. H., Cachau, R. E., Crowe, J., Davies, M., Kolaskar, A. S., Lund, O., Morrison, S., Mumey, B., Ofran, Y., Pellequer, J. L., Pinilla, C., Ponomarenko, J. V., Raghava, G. P., Van Regenmortel, M. H., Roggen, E. L. , Sette, A., Schlessinger, A., Sollner, J., Zand, M., Peters, B.(2007). Towards a consensus on datasets and evaluation metrics for developing B-cell epitope prediction tools. J. Mol. Recognit. 20(2), 75-82.

Kumar P., Gupta, A., Rajshekhar, Jayaraman, V. K. & Kulkarni, B.D. Aligning time series with genetically tuned dynamic time warping algorithm. Natural Computing Series of SPRINGER (edited by Z. Michalewicz and P. Siarry) (In Press).

Mundra, P. A., Madhan Kumar, Krishna Kumar, Jayaraman, V. K. & Kulkarni, B. D. Using Pseudo Amino Acid Composition to Predict Protein Subnuclear Localization: Approached with PSSM. Patt. Recognit. Lett. (In Press).

Kulkarni-Kale, U., Ojha, J., Manjari, S., Deobagkar, D. D., Mallya, A.D., Dhere, R. M. & Kapre, S. V. (2007). Mapping antigenic diversity & strain-specificity of mumps virus: a bioinformatics approach. Virology, 359, 436-446.

Gazal S., Krishnmurthy, S., Shah, V. & Kanhere, D. G. (2007). Density functional investigation of the interaction of acetone with small gold clusters. J. Chem. Phys. 126, 014704 .

2006

Kulkarni-Kale, U., Bhosle, S., Manjari, S., Joshi, M., Bansode, S. & Kolaskar, A. S. (2006). Curation of viral genomes: Challenges, applications and the way forward. BMC Bioinformatics, 7, S12.

Pandey, O. P. & Ghosh, I. (2006). Developing an antituberculosis compounds database and data mining in the search of a motif responsible for the activity of a diverse class of antituberculosis agents. J. Chem. Inf. Model. 46, 17-23.

Singh, V. K. & Ghosh, I. (2006). Kinetic modeling of tricarboxylic acid cycle and glyoxylate bypass in Mycobacterium tuberculosis, and its application to assessment of drug targets. Theor. Biol. Med. Model. 3, 27.

Ghosh, I. (2006). Target based High Throughput Screening and lead designing in pharmaceutical drug industry. Indian J. Chem. 45, 63-73.

* Idicula-Thomas, S., Kulkarni, A. J., Kulkarni, B. D., Jayaraman, V. K. & Balaji, P.V. (2006). A support vector machine-based method for predicting the propensity of a protein to be soluble or to form inclusion body on over expression in Escherichia coli. Bioinformatics, 22, 278 - 284.

Deshmukh, M. M., Gadre, S. R. & Bartolotti, L. J. (2006). Estimation of Intramolecular Hydrogen Bond Energy via Molecular Tailoring Approach. J. Phys. Chem. A. 110, 12519-12523.

Rangrez, A.Y., Dayananda, K.M., Atanur, S., Joshi, R., Patole, M.S. & Shouche, Y.S. (2006). Detection of Conjugation Related Type Four Secretion Machinery in Aeromonas culicicola, PLoS ONE, 1, e115.

Ghosh, S., Barve, A. C., Kumbhar, A. A., Kumbhar, A. S., Puranik, V.G., Datar, P. A., Sonawane, U. B. & Joshi, R.R. (2006). Synthesis, characterization, X-ray structure and DNA photocleavage by cis-dichloro bis(diimine) Co(III) complexes, J. Inorg. Biochem. 100, 331-343.

2005

Nagarajaram, H. A., Iengar, P. & Ghosh, I. (2005). In silico approach to antimalarial drug discovery: Design of selective inhibitor to Plasmodium falciparum aspartic proteases. Frontiers in Biophysics, 2005, 168-181.

Kulkarni-Kale, U., Bhosle, S. & Kolaskar, A. S. (2005). CEP: a conformational epitope prediction server. Nucl. Acids Res. 33, W168-W171.

Rajshekhar, Kulkarni, A., Jayaraman, V. K. & Kulkarni, B. D. (2005). Modeling Structure Property Relationships with Kernel Recursive Least Squares. Inter. Elect. J. Mol. Des. 4, 381-392.

Kumar R, Jayaraman, V. K. & Kulkarni, B. D. (2005). An SVM classifier incorporating simultaneous noise reduction and feature selection: Illustrative case examples. Patt. Recognit. 38, 41-49.

Kulkarni, O. C., Vigneshwar, R., Jayaraman, V. K. & Kulkarni, B. D. (2005). Identification of coding and non-coding sequences using local Hölder exponent formalism. Bioinformatics, 21, 3818-3823.

Jayaraman, V. K., Joshi, A., Chandran, S. & Kulkarni, B. D. (2005). Arrhythmia classification using local holder exponents and Support Vector Machines. Lect. Note. Comp. Sci. 3776, 242-247.

2004

Sarkar, D., Ghosh, I. & Datta, S. (2004). Biochemical characterization of Plasmodium falciparum HGXPRTase:role of histidine in substrate selectivity. Mol. Biochem. Parasitol. 137, 267-276.

Raychaudhury, C. & Ghosh, I. (2004). An Information-Theoretical Measure of Similarity and a Topological Shape and Size Descriptor for Molecular Similarity Analysis. Int. Elect. J. Mol. Des. 3, 350-360.

Kulkarni-Kale, U., Bhosle, S., Manjari, S., & Kolaskar, A. S. (2004). VirGen: A comprehensive viral genome resource. Nucl. Acids Res. 32, 289-292.

Kalate, R. N., Tambe, S. S. & Kulkarni, B. D. (2004). Designing optimum transcription efficiency experiments in eukaryotic systems using artificial intelligence. Bioinformatics India, 2, 22-33.

Shelokar, P. S., Jayaraman, V. K. & Kulkarni, B.D. (2004). An ant colony approach for clustering. Analyt. Chimica. Acta. 509, 187-195.

Shelokar, P. S., Jayaraman, V. K. & Kulkarni, B. D. (2004). An ant colony optimization–based classifier system for bacterial growth. Int. Elect. J. Mol. Des. 3, 572–585.

Kumar R., Kulkarni, A., Jayaraman, V. K. & Kulkarni, B. D. (2004). Symbolization assisted SVM classifier for noisy data. Patt. Recognit. Lett. 25, 495-504.

Kumar, R., Kulkarni, A., Jayaraman, V. K. & Kulkarni, B. D. (2004). Structure-activity relationships using locally linear embedding assisted by support vector and lazy learning regressors. Int. Elect. J. Mol. Des. 3, 118–133.

Kulkarni, D. Babu, K., & Gadre, S. R. (2004). Exploring hydration patterns of aldehydes and amides : Ab initio investigations. A. J. Phys. Chem. A. 108, 2492-2498.

Deshmukh, M., Sastry, N. V. & Gadre, S. R. (2004). Molecular Interpretation of Water Structuring and Destructuring effects: Hydration of Alkanediols. J. Chem. Phys. 121, 12402-12410.

Janaki, C. & Joshi, R. R. (2004) Motif detection in Arabidopsis: correlation with gene expression data. In Silico Biol. 4, 149-161.

2003

Awasthi, A., Mathur, R., Khan, A., Joshi, B. N., Jain, N., Sawant, S. Ramanamurthy, B., Mitr, D., & Saha, B. (2003). CD40 Signaling Is Impaired in L. major-infected Macrophages and Is Rescued by a p38MAPK Activator Establishing a Host-protective Memory T Cell Response. J. Exp. Med. 197, 1037-1043.

Kalate, R. N., Tambe, S. S. & Kulkarni, B. D. (2003). Optimizing transcription efficiency in eukaryotic systems using a hybrid approach involving an Artificial Neural Network and Genetic Algorithm: a case study of beta globin gene. WWW. J. Biol. 8, 82-98.

Kalate, R. N., Tambe, S. S. & Kulkarni, B. D. (2003). Artificial neural networks for prediction of mycobacterial promoter sequences. Comput. Biol. Chem. 27, 555-564.

Janaki, C. & Joshi, R. R. (2003). Accelerating comparative genomics using parallel computing. In Silico Biol. 3, 429-440.

2002

Sakharkar, M. K., Kangueane, P., Petrov, D. A., Kolaskar, A. S. & Subbiah, S. (2002). SEGE: A database on 'intron less/single exonic' genes from eukaryotes. Bioinformatics, 18, 1266-1267.

Saha, D. K., Padhye, S. B, Sinn, E. & Newton, C. (2002). Metal Complexes As Antitumor Agents 4: Synthesis, Structure, Spectroscopy and In Vitro Antitumor Activity of Hydroxynaphthoquinone Thiosemicarbazone Metal Complexes Against MCF-7 Human Breast Cancer Cell Lines. Ind. J. Chem. 41A.

Kalate, R. N., Kulkarni, B. D. & Nagaraja, V. (2002). Analysis of DNA curvature distribution in mycobacterial promoters using theoretical models. Biophys. Chem. 99, 77-97.

Cheema, J. J., Sankpal, N. V., Tambe, S. S. & Kulkarni, B. D. (2002). Genetic programming assisted stochastic optimization strategies for optimization of glucose to gluconic acid fermentation. Biotechnol. Prog. 18, 1356-1365.

WEST BENGAL UNIVERSITY OF TECHNOLOGY, KOLKATA

2007

Ghosh, K., Sarkar, S. & Bhaumik, K. (2007). Understanding image structure from a new multi-scale representation of higher order derivative filters. Image Vis. Comput. 25,1228-1238.

Ghosh, K., Sarkar, S. & Bhaumik, K. (2007). A theory of 'fuzzy' edge detection in the light of human visual system. J. Intell. Sys. (In press)

Aftabuddin, Md. & Kundu. S. (2007). Hydrophobic, hydrophilic and charged amino acids' networks within protein. Biophys. J. 93, 225-231.

2006

Ghosh, K., Sarkar, S. & Bhaumik, K. (2006). Proposing new methods in low-level vision from Mach band illusion in retrospect. Patt. Recog. 39, 726-730.

Ghosh, K., Sarkar, S. & Bhaumik, K. (2006). New vision tools from the comparative study of an old psychophysical model and a modern computation model. Biologically inspired approaches to advanced information technology: Springer Lect. Notes in Comput. Sci. 3853, 236-251.

Ghosh, K., Sarkar, S. & Bhaumik, K. (2006). Image enhancement by high order Gausian derivative filters simulating nonclassical receptive fields in human visual system. Pattern Recognition and Machine Intelligence: Springer Lect. Notes in Comput. Sci. 3776,453-448.

Ghosh, K., Sarkar, S. & Bhaumik, K. (2006). Early vision and image processing : evidences favouring dynamic receptive field model. Neural Information Processing: Springer Lect. Notes in Comput. Sci. 4338, 216-227.

Biswas, D., Roy, S. & Sen, S. (2006). A simple approach for indexing the oral druglikeness of a compound: Discriminating druglike compounds from nondruglike ones. J. Chem. Inf. Mod. 46, 1394-1401.

Roy, S. & Sen, S. (2006). Exploring the potential of complex formation between a mutant DNA and the wild type protein counterpart: A MM and MD simulation approach. J. Mol. Graph. Mod. 25, 158-168.

Aftabuddin, Md. & Kundu, S. (2006). Weighted and unweighted network of amino acids within protein. Physica A: Stat. Theor. Phys. 369, 895-904.

2005

Soumalee, B., Majumdar, R. & Bhattacharyya, D. (2005). Energy barriers and rates of tautomeric transitions in DNA bases: abinitio quantum chemical studies. Ind. J. Biochem. Biophys. 42, 378-385.

Roy, S. & Sen, S. (2005). Homology Modeling based solution structure of Hoxc8-DNA complex; role of context bases outside TAAT stretch. J. Biomol. Struct. Dyn. 22, 707-718.

2004

* Dasgupta, A. K., Majumdar, R. & Bhattacharyya, D. (2004). Characterization of non-planar peptide groups in protein crystal structures. Ind. J. Biochem. Biophys. 41, 233-240.

Ghosh, K., Sarkar, S. & Bhaumik, K. (2004). Edge enhancement in ultrasound images using biology inspired nonclassical centre-surround mechanism. J. Pure Appl. Ultrasonics, 26, 110-120.

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2007

Anuradha, A., Annadurai, R.S. & Shashidhara, L.S. (2007). Actin cytoskeleton as a putative target of the neem limonoid Azadirachtin A. Insect Biochem. Mol. Biol. 37, 627-634.

Praveen kumar, R., Manoj, M. N., Kush, A. & Annadurai, R.S. (2007). In silico approach of azadirachtin binding with actins. Insect Biochem. Mol. Biol. 37, 635-640.