

Dr. Hridoy Ranjan Bairagya

Present Address:

Dr. Hridoy Ranjan Bairagya,
Scientist Pool (C.S.I.R.,GOI)
Department of Biophysics
All India Institute of Medical Sciences
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Permanent Address:

Hridoy Ranjan Bairagya,
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Professional Experience: (Postdoctoral Research experience: 7 Years)

Scientist Pool (Senior Research Associateship funded by *Council of Scientific & Industrial Research*, Govt. of India) at Department of Biophysics, *All India Institute of Medical Sciences, New Delhi*, India. (2017 to date).

Research Associate (funded by *European Research Council*) at Department of Chemistry, *University of Cambridge*, UK in the group of **Prof. David J. Wales** (2015 to 2016).

Young Scientist/PI (funded by of *Science and Engineering Research Board*, Govt. of India) at Molecular Biophysics Unit, **Indian Institute of Science-Bangalore**, India in the group of **Prof. Manju Bansal** (2013 to 2015).

Post Ph.D. Research Fellow at Department of Chemistry, *National Institute of Technology – Durgapur*, India in the group of **Prof. Bishnu Prasad Mukhopadhyay** (2012 to 2013).

Ph.D research experience (2006 to 2012)

Senior Research Fellow (funded by *Council of Scientific & Industrial Research*, Govt. of India) at Department of Chemistry, National Institute of Technology –Durgapur, India, in the group of **Prof. Bishnu Prasad Mukhopadhyay** (2010 to 2012).

Academic Qualifications:

Ph.D. in Engineering in Biotechnology (specialization *Bioinformatics*) from National Institute of Technology-Durgapur, Govt. of India, 2012.

M.Sc. in Bioinformatics from Sikkim Manipal University of Health, Medical & Technological Sciences, India, 2004.

B.Sc. in Zoology (Honours) from Burdwan University, India, 2002.

Certificate Course: PLT using platform independent language (**JAVA**) from Score Information Technologies Limited (Software training institute) Kolkata (2Camac Street), India, 2004

✓ **Teaching Experience: (experience: More than 2 Years)**

Expert lectures for Biotechnology of Semester I students at Department of Biotechnology, **Visva-Bharati University (Central University)**, **Santiniketan** 731235, and West Bengal, India.

Guest Faculty (Assistant Professor) in **M.Sc. Bioinformatics** course at Department of Computer Science in **Central University**, Jamia Millia Islamia -New Delhi, from 2018 to date.

Subject taught: 2018 to date

Semester	Paper Title	Paper Code	Credits
III	Computational Methods for Data Analysis	MB-32	4
III	Lab-VI (Bioinformatics Tools-III)	MB36	2
I	Lab-I (Bioinformatics Tools + R Language)	MB1816	2
II	Structural Bioinformatics	MB1824	4
II	Lab-IV (Advance Bioinformatics Tools-II)	MB1827	2
III	Simulation Techniques in Bioinformatics	MB1835	4

Research Techniques:

Computational Molecular Dynamics Simulation: MD simulation study of large proteins, enzyme–substrate complexes, protein–ligand complexes, protein-metal complexes and RNA-peptide complexes. pH dependent MD simulation study of enzyme to mimic experimental methods. Water molecular dynamics of macromolecules. Conformational dynamics of RNA-peptide complexes. Loop-flap molecular dynamics study of protein. Binding free energy calculation of ligand by MM (GB)PB methods. Thermal denaturation of ribozyme. Force field parameterization of new ligands.

Computational Structural Bioinformatics: Protein engineering, Prediction of 3D structure of protein and loop of the protein structure by homology modeling, energy minimization and molecular dynamics simulation study. Modeling the ternary complex of metallo proteins. Inter domain recognition process of macromolecules. Identifying and modeling the key water molecules in protein and protein-ligand complexes. Prediction the flexibility and functional role of water molecules. Methods for pocket monitoring during MD simulation.

Structure refinement and Protein Crystallography: Structure prediction of protein and protein-ligand complexes using molecular replacement method. **Protein structures (**PDB Id: 5YIH, 5YL8, 5YRR, 6A31, 5ZZV, 6A89 and 6LSO**) deposited at Protein DataBank.

Computational Biochemistry: Purine nucleotide biosynthesis pathway analysis. Activity and mechanism of enzyme. Conformational transition of enzyme from ligand free to ligand bound state. Prediction the functional role of non catalytic residues of enzyme – substrate complexes. Identification of allosteric site of the enzyme. Subsite site recognition of ligands.

Computational Charge transfer mechanism: Water mediated electron transfer mechanism of metalloprotein, water mediated charge transfer mechanism within salt bridges of protein.

Molecular modeling and Docking study: Prediction the model structure of new ligand and modification of existing ligand on the basis of ligand–water interaction. Database development of new ligands. Molecular docking study of protein-protein, protein-inhibitor, protein-ligand and protein-drugs.

Computer aided drug discovery: Design of inhibitors for Chronic myeloid leukemia (CML) and TTR (Transthyretin) associated amyloid diseases. Salt Bridge based drug discovery, water based drug discovery, structure based drug discovery, enzymatic mechanism based drug discovery. Virtual screening from ligand database, QSAR and ADMET Properties Prediction.

Experience on disease: Blood cancer (Chronic myeloid leukemia (CML) cancer on human IMPDH depended pathway), TTR (Transthyretin) associated amyloid diseases and arthritis.

Computational Genomics: Prediction of gene from genome using codon adaptation index (CAI).

Experience on Biomolecular system:

Enzymes/proteins: Human Inosine monophosphate dehydrogenase (hIMPDH), Human Guanine Monophosphate Synthetase (hGMPS), Human Matrix metalloproteinases (hMMPs), Plant cysteine proteases and Human Transthyretin.

Metalloprotein: Rusticyanin (RCy), Cytochrome (Cyt c4), and Cytochrome oxidase (CcO).

Nucleic acids: Full length hammerhead ribozyme and HIV trans-activation response (TAR) RNA

Skills and Knowledge:

System Skills: Clusters/Supercomputers and GPU based Workstation

Operating System: Linux/Unix and Windows

High performance Computing (HPC) for Molecular Dynamics Simulation of Biomolecules:

The molecular dynamics simulation of large biomolecule (enzymes, protein-ligand complexes, ribozyme, RNA-peptide complexes) was carried out on different GPU based workstations and as well as linux Cluster using the AMBER and NAMD simulation packages.

Software Knowledge:

Molecular Dynamics Simulation Packages: NAMD (Nanoscale Molecular Dynamics), AMBER

Biomolecular visualizing and editing packages: Swiss PDB Viewer, DS-Visualizer, Visual Molecular Dynamics (VMD) program and its associate analysis tools, Auto IMD, FOLDX program, POPS*program, Hyperchem program, Adaptive Poisson–Boltzmann Solver (APBS) program, CHASA program, ProACT2 (Protein Accessibilities, CaviTies and ConTacts) program.

Docking, Toxicology and QSAR packages: Autodok program, different web based docking programs, AuDocker, Molinspiration program, OSIRIS property explorer program.

Protein Structure refinement packages: Win-Coot, CCP4i and Crystallography and NMR system (CNS).

Statistical Package: Matlab -2011 and R

Programming language: C, C⁺⁺, TCL scripting, Python, Perl and Java

Research Experience:

Independent (Scientist's Pool Scheme by CSIR) Research Experience: (2017 to date)

Title of the work: “Understanding the structure and mechanism of human Guanosine Monophosphate Reductase (GMPR) enzyme: A study towards the design of anticancer agent” at Department of Biophysics, All India Institute of Medical Sciences, in the group of Structural Bioinformatics and Protein Crystallography.

Post Doctoral Research Experience: (2015 to 2016)

Title of the work: “The cold denaturation of full-length hammerhead ribozyme: A study by MD simulation methods” and “Binding affinity of tri peptide ligands to TAR-RNA: A study by MD simulation approaches” at Department of Chemistry, University of Cambridge in the group of computational Chemistry.

Post Doctoral Research Experience: (2013 to 2015)

Title of the work “Molecular Dynamic Simulation study on human Guanosine Monophosphate Synthetase (GMPS) enzyme and their hydrated complex: A theoretical approach towards the design of anticancer agent” at Indian Institute of Science-Bangalore, Molecular Biophysics Unit, India, **Post Ph.D.**

Research experience (2012 to 2013)

“Water mediated salt bridge interaction and role of carboxamide group of NAD⁺ in hIMPDH enzyme: A study by MD-Simulation method” at National Institute of Technology –Durgapur, Department of Chemistry, India.

Ph.D. Research experience (2006 to 2012)

Title of thesis “A study on the Role of Conserved Water Molecules in Human Inosine Monophosphate Dehydrogenase (hIMPDH) Enzyme by Molecular Dynamics Simulation Methods” at National Institute of

Technology –Durgapur, Department of Chemistry, India.

P.G. Research experience (2004 to 2004)

Title of P.G. thesis: “Signature of the Chloroplast gene in Cyanobacteria” Department of Biophysics, Molecular Biology & Genetics, University of Calcutta, India.

Experience of PG thesis guidance: 04

Academic Achievement:

Fellowship:

1. Received award from Institute Research Fellowship from National Institute of Technology – Durgapur, Govt. of India, for the period 2006 – 2010.
2. Received award from the Council of Scientific and Industrial Research (CSIR, Govt. of India), Senior Research Fellowship for the period 2010 - 2012.
3. Recipient of a “**Young Scientist**” award from Science and Engineering Research Board (Govt. of India), 2013 to 2015.
4. Received award from the Council of Scientific and Industrial Research (CSIR, Govt. of India), Senior Research Associateship (**Scientist’s Pool scheme**) for the period 2017 - 2020.

Awards:

1. Received Foreign travel Grant from C.S.I.R., Govt. of India on 2009.
2. Received Foreign travel Grant from C.S.I.R., Govt. of India on 2011.
3. Bruker Axs India Best Poster Award: In 2008, “37th National Seminar on Crystallography “, held at Jadavpur university one of our research work “Invariant Water Molecular Dynamics at the catalytic site of IMPDH II “Bruker Axs India Best Poster Award.

Invited scientific talk:

- **Speaker and resource person** on National Seminar of “Recent Trends in Pharma Biotechnology” at Department of Biotechnology, IILM College of Engineering & Technology, Greater Noida, UP on September 17th, **2019**.

- **Keynote Speaker** (Title: “New insights into the dynamics of enzyme and nucleic acids: Computational approaches for conserved water based drug discovery”) **at National Workshop (9th) on Translational Bioinformatics** at Department of Computer Science, Jamia Millia Islamia, New Delhi from 6th March to 7th March, **2019**.
- **Speaker and resource person** of the program "Approaches for In silico drug designing" sponsored by A.P.J. **Abdul Kalam Technical University**, on July 3-7, **2018** at Department of Biotechnology at IILM College of Engineering & Technology, Greater Noida, UP.
- Deliver the invited scientific talk on “*New insights into the dynamics of enzyme and nucleic acids: Computational approaches for conserved water based drug discovery*” at Department of Biotechnology, Siksha, Bhavana, **Visva-Bharati University** (Santiniketan-731235) dated on 6th March, 2017.
- Delivered the **scientific talk** at Albany, USA in the “The 17th Conversation “on June 14-18, 2011, State university of New York, USA in the **Young Scientists Speaker** Program.
- Deliver Scientific talk at 40th National Seminar on Crystallography–2011 (Osmania University, Hyderabad, India) dated 23rd – 25th October, **2011**.

Major Research Projects (two) as PI:

1.

- **Project Title:** “Understanding the structure and mechanism of human Guanosine Monophosphate Reductase (GMPR) enzyme: A study towards the design of anticancer agent”.
- **Period of Operation:** 2017 to 2020
- **Host Institute:** Department of Biophysics, All India Institute of Medical Sciences, New Delhi-110029, INDIA
- **Sponsoring Agency:** Council of Scientific and Industrial Research (CSIR, Govt. of India.)
- **Purpose of the award:** The Senior Research Associateship / Scientist’s Pool scheme is a primarily meant to provide temporary placement to highly qualified Indian scientists (below the age of **40** years) returning from abroad, who are not holding any employment in India. It is not a regular appointment, but is a temporary facility to enable the Associate to do research/teaching in India while looking for a regular position.
- **Nature of Award:** Each award carries an amount of Rs.21,000 to Rs.25,810 per month (fixed) with other benefits being paid to Pool Scientist as a fellowship and other grants on the above research project for a period of three Years.

2.

- **Project Title:** “Molecular dynamic simulation study on human guanosine monophosphate synthetase(GMPS) enzyme and their hydrated complex: A theoretical approach towards the design of anticancer agent”.
- **Period of Operation:** 23-09-2013 to 30-06-2015
- **Host Institute:** Molecular Biophysics Unit, Indian Institute of Science-Bangalore, PIN-560 012.

- **Sponsoring Agency:** Science and Engineering Research Board, D.S.T., Govt. of India.
- **Purpose of the award:** It was instituted to provide research funding to the “**Young Scientist**” below the age of 35 years to undertake independent research in newly emerging and frontier areas of Science and Engineering.
- **Nature of Award:** Each award carries an amount of Rs 35,000/- pm (revised Rs.55,000/-pm), is being paid to Young Scientist as a fellowship on the above research project and a total research grant of Rs. 18 lakhs for a period of three Years.

International Research Project: The research proposal “*Novel application of energy landscapes methodology to analyze conformational transitions and binding pathways of HIV-I TAR-RNA with TAT protein and other potential inhibitors*” submitted under *Marie Skłodowska-Curie* actions fellowship (2016), was scored *as a high-quality* project proposal in a highly competitive evaluation process. This proposal is recommended for funding by other sources since Horizon 2020 resources.

Reviewer of the Journal: Microbial Pathogenesis, Journal of Biomolecular Structure and Dynamics and Journal of Molecular Modeling.

Member of Editorial Board:

- i. International Journal of Molecular Biology and Biochemistry (IJMBB)
- ii. Advances in Applied Mathematical Biosciences (AAMB)
- iii. Bioinformatics & Proteomics Open Access Journal (BPOJ)

Professional Recognitions:

- i. Life Member of **Indian Crystallographic Association:** (LM284)
- ii. Life Member of **Indian Biophysical Society:** (LM 634)
- iii. Life Member of **Society of Biological Chemists:** (Life Memb. NO.: 2582)

Publications in International peer-reviewed scientific journals:

[Total publications: 34, **Total Citations: 250 and h-index:8]

1. Hridoy R. Bairagya*

Conformational Transition of Catalytic Domain in hGMPR enzyme from Native to Ligand Bound State: A MD Simulation Study.

J. Biomolecular Structure & Dynamics, 37(S1), 66-67, 2019.

2.Hridoy R. Bairagya*, Alvea Tasneem, Gyan Prakash Rai, Saima Reyaz.

Role of conserved water molecules at GMP binding domain in native conformation of human GMPR enzyme: A MD simulation study. **Proceedings at National Workshop (9th) on Translational Bioinformatics, 2019.**

3. Hridoy R. Bairagya* and Manju Bansal

New insight into the architecture of oxy-anion pocket in unliganded conformation of GAT domains: A MD-Simulation Study. **Proteins: Structure Function and Bioinformatics**, 84, 360–373, **2016**.

4. Hridoy R. Bairagya, Deepak K. Mishra, Bishnu P. Mukhopadhyay* and K. Sekar

Conserved water-mediated recognition and dynamics of NAD⁺ (carboxamide group) to hIMPDH enzyme: water mimic approach toward the design of isoform-selective inhibitor

J. Biomolecular Structure & Dynamics, 32(8), 1248-1262, **2014**.

5. Hridoy R Bairagya and Bishnu P Mukhopadhyay*

Protein folding: challenge to chemistry.

J. Biomolecular Structure & Dynamics, 31(9), 993-994, **2014**.

6. Hridoy R Bairagya and Bishnu P Mukhopadhyay*

An Insight to the Dynamics of Conserved Water Mediated Salt Bridge Interaction and Inter-Domain Recognition in hIMPDH Isoforms. **J. Biomolecular Structure & Dynamics**, 31(7), 788-808, **2013**.

****Cited in Proteopedia as Interactive 3D Complements from Weizmann Institute of Science, Israel.**

7. Hridoy R Bairagya, Bishnu P Mukhopadhyay*, and Asim K Bera

Role of Salt bridge Dynamics in inter domain recognition of Human IMPDH Isoforms: An Insight to inhibitor Topology for isoform –II. **J. Biomolecular Structure & Dynamics**. 29, 441-462, **2011**.

8. Hridoy R Bairagya, Bishnu P Mukhopadhyay*, Payel Mallik, Archana K. Srivastava

Conserved Water Mediated H-bonding Dynamics of Carboxamide group in NAD to Catalytic Asp 274 and His 93 in Human IMPDH **J. Biomolecular Structure & Dynamics**, 28,1008-1010, **2011**.

9. Hridoy R Bairagya, Bishnu P Mukhopadhyay* and Asim K Bera

Conserved Water Mediated Recognition and the Dynamics of Active site Cys 331 and Tyr 411 in Hydrated Structure of Human IMPDH-II. **Journal of Molecular Recognition**, 35 - 44, 24, **2011**.

10. Hridoy R Bairagya, Bishnu P Mukhopadhyay* and K. Sekar

An Insight to the Dynamics of Conserved Water Molecular Triad in **IMPDH II** (Human): Recognition of Cofactor and Substrate to Catalytic Arg 322.

J. Biomolecular Structure & Dynamics 27, 2, 149 – 158, **2009**.

11. Hridoy R Bairagya, Bishnu P Mukhopadhyay* and S. Bhattacharjee
Role of the conserved water molecules in the binding of inhibitor to **IMPDH-II**
(human): A study on the water mimic inhibitor design .
Journal of Molecular Structure:THEOCHEM 31-39, 908, **2009**.

12. Hridoy R Bairagya, Bishnu P Mukhopadhyay*
Conserved Water Mediated Inter-Domain Recognition in IMPDH-II (human).
The 16th Conversation: at the State University of New York, Albany ,
J. Biomolecular Structure & Dynamics 26: 855, **2009**.

13. Sanchita Banerjee, Ankit Roy, M S Madhusudhan, **Hridoy R Bairagya** and Amit Roy*

Structural insights of a cellobiose dehydrogenase enzyme from the basidiomycetes fungus *Termitomyces clypeatus*. **Journal of Computational Biology and Chemistry (Accepted)**, **2019**.

14. Hridoy R Bairagya, Bishnu P Mukhopadhyay* and K. Sekar
Conserved Water Mediated H-bonding Dynamics of Inhibitor, Cofactor, Asp 364 and Asn 303 in Human IMPDH II. **J. Biomolecular Structure & Dynamics**, 26,4, 497-508, **2009**.

15. Varun Kumar, P. Sharma, **H.R. Bairagya**, S. Sharma, T P Singh, Purnima Kaul Tiku,
Inhibition of human 3-hydroxy-3-methylglutaryl CoA reductase by peptides leading to cholesterol homeostasis through SREBP2 pathway in HepG2 cells. **BBA - Proteins and Proteomics**, 1867, 604-615, **2019**.

16. A.Gupta, P.K.Singh, N.Iqbal, P.Sharma, **H.R.Baraigya**, P.Kaur, M.S.Umar, F.Ahmad, A.Sharma, M.Owais, S. harma, T.P.Singh*

Structural and binding studies of Phosphopantetheine adenylyl transferase from *A. baumannii* with citric and ascorbic acid. **BBA - Proteins and Proteomics**, 1867 (6), 537-547, **2019**.

17. P. Dey, **Hridoy R Bairagya** and Amit Roy*
Putative role of invariant water molecules in the X-ray structures of family G fungal endoxylanases
Journal of Biosciences, 43 (2), 339-349, **2018**.

18. A. Chaudhary, V Kumar, P. K. Singh, P. Sharm, **Hridoy R. Bairagyaa**, P. Kaur, S. Sharma, S. S. Chauhan, T. P. Singh*
A glycoprotein from mammary gland secreted during involution promotes apoptosis: Structural and biological studies. **Archives of Biochemistry and Biophysics**, 644,72-80, **2018**.

19. Prashant K. Singh, Naseer Iqbal, Harsh V.Sirohi, **Hridoy R.Bairagya**, Punit Kaur, Sujata Sharma, Tej P.Singh*. Structural basis of activation of mammalian heme peroxidases. **Progress in Biophysics and Molecular Biology**, 133,4 9-55, **2018**.

20. B. Chakrabarti, **Hridoy R. Bairagya**, Bishnu P Mukhopadhyay* and K.Sekar
New biochemical insight of conserved water molecules at catalytic and structural Zn^{+2} ions in Human Matrix Metalloproteinase-I: A Study by MD-Simulation. **Journal of Molecular Modelling**, **23(2): 57, 2017.**
21. Avik Banerjee, **Hridoy R Bairagya**, Bishnu P Mukhopadhyay*, Tapas K Nandi, Deepak K Mishra
Conserved water mediated H-bonding dynamics of Ser 117 and Thr 119 residues in human transthyretin - thyroxin complexation: Inhibitor modeling study through docking and molecular dynamics simulation
Journal of Molecular Graphics and Modelling, **44, 70-80, 2013.**
22. Bornali Chakrabarti, **Hridoy R Bairagya**, Deepak K Mishra, Pradip Kumar Chatterjee, Bishnu P Mukhopadhyay*
Insight towards the conserved water mediated recognition of catalytic and structural Zn^{+2} ions in human Matrix Metalloproteinase-8 enzyme: A study by MD-simulation methods. **Bioinformation**, **126-133, 9(3), 2013.**
23. Deepak K, Mishra, Bishnu P. Mukhopadhyay*, **Hridoy R. Bairagya**
Molecular Modeling of Inosine 5'-Monophosphate Dehydrogenase-II (Human) Structure using MD simulation methods. **International Journal of Pharma and Bio Sciences** 3(4): (B) 102 – 120, **2012.**
24. Tapas K Nandi, **Hridoy R Bairagya**, Deepak K Mishra, Bishnu P Mukhopadhyay*, Avik Banerjee
Structural and Putative Functional Role of Conserved Water Molecular Cluster in the X- ray structures of Plant Thiol Proteases: A Molecular Dynamics Simulation Study. **Journal of Chemical Crystallography** 42(11), 1105-1118, **2012.**
25. Tapas K Nandi, **Hridoy R Bairagya**, Bishnu P Mukhopadhyay*, Payel Mallik, Dipankar Sukul and Asim K Bera
Conserved water mediated H-bonding dynamics of catalytic His 159 and Asp158 : An insight to possible acid – base coupled mechanism in plant thiol protease.
Journal Molecular Modeling 18(6), 2633-2644, **2012.**
26. B.Ghosh, Bishnu .P. Mukhopadhyay*, **Hridoy R. Bairagya**
Effect of amino acids on bioleaching of chalcopyrite ore by Thiobacillus ferrooxidans.
African Journal of Biotechnology 11(8), 1991-1996, **2012.**
27. Bornali Chakrabarti , **Hridoy R Bairagya***, Payel Mallik , Bishnu P Mukhopadhyay and Asim K Bera
An Insight to Conserved Water Molecular Dynamics of Catalytic and Structural Zn^{+2} ions in Matrix Metalloproteinase 13 of Human.
J. Biomolecular Structure & Dynamics 503 – 516 , 28 (4), **2011.**
28. Avik Banerjee, **Hridoy R Bairagya**, Bishnu P Mukhopadhyay*, Tapas K Nandi
Role of Conserved Water molecules in binding of Thyroxin and analogs inhibitors to human Transthyretin: A study on water-mimic inhibitor design
J. Biomolecular Structure & Dynamics, 28, 1027-1028, **2011.**

29. Bishnu P Mukhopadhyay* and Hridoy R Bairagya

Protein Folding: Grand Challenge of Nature. **J. Biomolecular Structure & Dynamics** 337 – 338, 28 (4), **2011**.

30. Avik Banerjee, Hridoy R Bairagya, Bishnu P Mukhopadhyay*, Tapas K Nandi and Asim K Bera

Structural insight to mutated Y6S transthyretin by molecular dynamics simulation

Indian Journal of Biochemistry & Biophysics 47 (4)197 – 202, **2010**.

31. Tapas K Nandi, Hridoy R Bairagya, Bishnu P Mukhopadhyay*, D . Sukul, A.K.Bera and K. Sekar

Conserved water-mediated H-bonding dynamics of catalytic Asn 175 in plant thiol protease.

J. Biosciences, (34) 27–34, **2009**.

32. B.P.Mukhopadhyay*, B.Ghosh, H.R.Bairagya, T.K.Nandi, B.Chakrabarti and A.K.Bera

Molecular Modeling of the Ternary Complex of Rusticyanin -Cytochrome c4 –Cytochrome oxidase : An Insight to Possible H- Bond Mediated Recognition & Electron Transfer Reaction in *T. ferrooxidans*

J. Biomolecular Structure & Dynamics, 25,5, 543- 552, **2008**.

33. B.P.Mukhopadhyay*, B.Ghosh, H.R.Bairagya, A.K.Bera , T.K.Nandi and S.B. Das

Modeling Study of Rusticyanin-Cytochrome C4 Complex: An Insight to Possible H-Bond Mediated Recognition and Electron Transfer Process?

J. Biomolecular Structure & Dynamics , 25, 2, 157- 164, **2007**.

34. B.P.Mukhopadhyay*, B.Ghosh, H.R.Bairagya, A.K.Bera and R.K.Roy

Conserved Water Molecular Dynamics of the Different X-ray Structures of Rusticyanin: An Unique Aqueation Potentiality of the Ligand Bonded Cu⁺⁺ Center.

J. of Biomolecular Structure & Dynamics, 24, 4, 369- 378, **2007**.

Manuscript under preparation: 1. Binding stability of tri peptides ligands to TAR RNA: A study by MD simulation and energy landscape methods (2018).

List of Papers presented in International Conference: (07)

1. **Hridoy R. Bairagya*** and Tej. P. Singh

New structural insight of GMP binding domain in unliganded conformation of hGMPPR enzyme: A MD simulation study.

Multiscale Simulation & Mathematical Modelling of Complex Biological Systems from 30-01-2019 to 1-02-2019 at Jawaharlal Nehru University, New Delhi, India.

2. Deepak K. Mishra, **Hridoy R. Bairagya** and Bishnu P. Mukhopadhyay

Role of conserved water molecular triad in the recognition of IMP,NAD⁺ with Asp 274, Asn 303, Arg322, and Asp 364 in both the isoform of hIMPDPH.

State University of New York, Albany 2013: **The 18th Conversation**, June -2013.
31 (S1),111, 2013.

3. **Hridoy R Bairagya** , Bishnu P Mukhopadhyay and Sunav Dutta.

The Invariant Aquation Potentiality of the Active site Residues of Human IMPDH II.

International Conference on Bioinformatics. December 20th -22th, 2007 at University of Hyderabad.

4. B.Ghosh, B.P.Mukhopadhyay and **H.R.Bairagya**

Invariant water molecular interaction in the acidophilic redox protein Rysticyanin of Thiobacillus ferroxidans.

International Symposium on Computational Biology & Bioinformatics (ISBB 06) 15th -17th December 2006 at Bhubanswar.

5. B.Ghosh, B.P.Mukhopadhyay and **H.R.Bairagya**

Modeling studies of the Rysticyanin –Cytochrome C4 Complex Involving in the Thiobacillus ferroxidans During the Electron Transfer Reaction.

International Symposium on Computational Biology & Bioinformatics. (ISBB 06) 15th -17th December 2006 at Bhubanswar.

6. Bishnu P Mukhopadhyay and **Hridoy R Bairagya**

Molecular Dynamics Study of IMPDH II (Inosine Monophosphate Dehydrogenase) and its Complexes : A Probe to Design Potent Anticancer Agents / Inhibitors.

International Symposium on Recent Trends in Macromolecular Structure and Function (“ISRTMSF 2008”) at Madras University, 7th – 11th January, 2008.

7. Bishnu P Mukhopadhyay ,**Hridoy R Bairagya** and B. Chakrabarti

Molecular Dynamics Study of Matrix Metalloproteinase (MMP - 13) : An Insight to Hydration Propensity at Active Zn⁺² site.

International Symposium on Recent Trends in Macromolecular Structure and Function (“ISRTMSF 2008”) at Madras University, 7th – 11th January, 2008.

List of Papers presented in National Conference: (23)

1. Gyan Prakash Rai and Hridoy R. Bairagya*

New structural insight of GMP binding domain in unliganded conformation of hGMMPR enzyme: A MD simulation study. **National Workshop (9th) on Translational Bioinformatics** at Department of Computer Science, Jamia Millia Islamia, New Delhi from 6th March to 7th March, 2019.

2. Saima Reyaz and Hridoy R. Bairagya*

Structural and functional role salt bridges in catalytic domain of human GMMPR enzyme: A study by MD simulation method. **National Workshop (9th) on Translational Bioinformatics** at Department of Computer Science, Jamia Millia Islamia, New Delhi from 6th March to 7th March, 2019.

3. Alvea Tasneem and Hridoy R. Bairagya*

Role of Conserved Water Molecules in Nucleotide Binding Domain of hGMMPR Enzyme: MD simulation study. **National Workshop (9th) on Translational Bioinformatics** at Department of Computer Science, Jamia Millia Islamia, New Delhi from 6th March to 7th March, 2019.

4. Hridoy R.Bairagya* and Manju Bansal

New insight to oxyanion hole in unliganded conformation of GAT domain: Understanding the role of water molecules.
83rd Annual Meeting of **Society Of Biological Chemists (India)**, held on December 17th to 21st, 2014 at KIIT-University.

5. Hridoy R.Bairagya and Manju Bansal

Water mediated recognition of catalytic His190 in GAT domain: New insight from molecular dynamics simulations.
Annual Conference of Indian Biophysical Society entitled "Molecular Architecture, Dynamics and Assembly in Living Systems" 7th -10th February, 2014, at Saha Institute of Nuclear Physics- Kolkata.

6. Hridoy R.Bairagya and Bishnu P. Mukhopadhyay

Recognition of Gln36 and Thr152 in GATse domain of hGMPS enzyme: An investigation by M.D. Simulation. **42 National Seminar on Crystallography**, November 21st to 23rd, 2013 at Department of Biophysics, All India Institute of Medical Sciences-New Delhi.

7. H. R. Bairagya and B. P. Mukhopadhyay

The design of isoform specific anti leukemic agent using conserved water Molecular Dynamics of human IMPDH.

40th National Seminar on Crystallography, 26th-28th November, 2011. Department of Physics, Osmania University, Hyderabad.

8. A. Banerjee, **H. R. Bairagya**, D. K. mishra and B. P. Mukhopadhyay

Dynamics of Conserved Water Molecules in the Thyroxine binding region of Human transthyretin: A MD Simulation study.

40th National Seminar on Crystallography, 26th -28th November, 2011. Department of Physics, Osmania University, Hyderabad.

9. B. Chakrabarti, **H. R. Bairagya** and B. P. Mukhopadhyay

Conserved Water Molecular Dynamics of Catalytic and Structural Zn²⁺ ions in Human Matrix Metalloproteinase I.

40th National Seminar on Crystallography, 26th -28th November, 2011. Department of Physics, Osmania University, Hyderabad.

10. T. K. Nandi, **H. R. Bairagya** and B. P. Mukhopadhyay

Role of conserved water chain / cluster in plant thiol proteases: A Molecular Dynamics Simulation Study.

40th National Seminar on Crystallography, 26th -28th November, 2011. Department of Physics, Osmania University, Hyderabad.

11. B.P.Mukhopadhyay and **Hridoy R Bairagya**

Water Molecular Dynamics of IMPDH: A Step towards the CML-specific Inhibitors Design.

IIIrd National Conference On New Frontiers In Haematology & Oncology at Netaji Subhas Chandra Bose Cancer Research Institute, Kolkata from Sept. 11st -12th, 2010.

12. **H. R. Bairagya** and B. P. Mukhopadhyay

Conserved Water Mediated Inter-domain Recognition and Dynamics of Human IMPDH isoforms: An insight to antileukemic drug selectivity.

80th annual meeting of the Society of Biological Chemists (SBS) at Central Institute of Medicinal and Aromatic Plant (CIMAP), Lucknow dated on Nov. 12th – 15th, 2011.

13. B. P. Mukhopadhyay and **H. R. Bairagya**

Conserved Water Mediated Recognition in human IMPDH: Water Mimic Drug Design in CML Cancer.

80th annual meeting of the Society of Biological Chemists (SBS) at Central Institute of Medicinal and Aromatic Plant (CIMAP), Lucknow dated on Nov. 12th – 15th, 2011.

14. B.P.Mukhopadhyay and **Hridoy R Bairagya**

Water Molecular Dynamics and Recognition of Inosine Monophosphate Dehydrogenase (IMPDH)- II in Human: Hope and Scope For AntiCancer Drug Design.

Symposium On Recent Trends In Biophysics and Workshop On Emerging Techniques of Biophysics at Banaras Hindu University, Varanasi from Feb. 13th -16th, 2010.

15. **Hridoy R Bairagya** and B.P.Mukhopadhyay

Conserved Water Mediated Inter-Domain Recognition in IMPDH- II (Human) **Symposium On Recent Trends In Biophysics and Workshop On Emerging Techniques of Biophysics** at Banaras Hindu University, Varanasi from Feb. 13th -16th, 2010.

16. B.P.Mukhopadhyay and **Hridoy R Bairagya**

Conserved water based inhibitor designing of human IMPDH- II: The New strategy in Structural Biology. **38th National Seminar On Crystallography**, NSC-38 at University of Mysore, from Feb. 11th– 13th, 2009.

17. Avik Banerjee, **Hridoy R Bairagya** and B.P.Mukhopadhyay

Structural insight to mutated Y116S Transthyretin by molecular dynamics simulations. **38th National Seminar On Crystallography**, (NSC-38) at University of Mysore, from Feb. 11th – 13th, 2009.

18. B. Chakrabarti , **Hridoy R Bairagya** and B. P.Mukhopadhyay

Catalytic Role of the Structural Zn²⁺ through water molecular coordination: A New Insight to MMP 13 Collagenolytic Activity. **38th National Seminar On Crystallography**, (NSC-38) at University of Mysore, from Feb. 11th–13th, 2009.

19. **Hridoy R Bairagya** , Sunav Dutta and Bishnu P Mukhopadhyay

Modeling the IMPDH-II receptor in human for designing the anticancer inhibitor using MD –simulation studies. **National Symposium on Cellular and Molecular Biophysics**, (NCMB-2009), dated 22nd -24th Jan., 2009 at Centre for Cellular and Molecular Biology, Hyderabad .

20. B. P. Mukhopadhyay, **H. R. Bairagya** and T. K. Nandi

Molecular Modeling of the Ternary Complex of Rusticyanin -Cytochrome c4 –Cytochrome oxidase. **37th National Seminar On Crystallography** , (NSC-37) at Jadavpur university, 6th – 8th February, 2008

21. **Hridoy R Bairagya**, B. Chakrabarti and Bishnu P Mukhopadhyay

Invariant Water Molecular Dynamics at the Catalytic-site of IMPDH II (Inosine Monophosphate Dehydrogenase).

37th National Seminar On Crystallography, (NSC-37) at Jadavpur University, 6th – 8th February, 2008.

22. B.P.Mukhopadhyay, **H.R.Bairagya** and B.Ghosh

Cu⁺² leaching from Chalcopyrite ore by *Thiobacillus ferrooxidans* in presence of amino acids.

National Seminar on Mineral Biotechnology, (NSMB 2007), 30th – 31st Jan, 2007. Regional Research Laboratory (RRL) CSIR, Bhubanswar, Orissa.

23. B.P.Mukhopadhyay, **H.R.Bairagya** and B.Ghosh

Modeling study of Rusticyanin - Cytochrome C₄ Complex Modeling of Human IMPDH Type I Enzyme: Computational Structure Prediction of Protein.

National Seminar on Mineral Biotechnology, (NSMB 2007), 30th – 31st Jan, 2007. Regional Research Laboratory (RRL) CSIR, Bhubanswar, Orissa.

References:

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