

AKASH DEEP BISWAS

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RESEARCH PUBLICATIONS

Published in Peer Reviewed International Journal

- ❖ Vinod Kumar Yata, Shweta Mahajan, Arun Thapa, Shadab Ahmed, **Akash Deep Biswas**, Airy Sanjeev, and Venkata Satish Kumar Mattaparthi. "In silico methods reconfirm CDK2 as a potential molecular target of 5-fluorouracil", Indian Journal of Biochemistry and Biophysics (2016)
<http://nopr.niscair.res.in/bitstream/123456789/42643/1/IJBB%2053%285%266%29%20199-205.pdf>
- ❖ Bandana Bora, **Akash Deep Biswas**, Arun Bahadur Gurung, Atanu Bhattacharjee, Mattaparthi Venkata Satish Kumar, and Ashis K. Mukherjee. "An in silico approach to understand the structurefunction properties of a serine protease (Bacifrinase) from *Bacillus cereus* and experimental evidence to support the interaction of Bacifrinase with fibrinogen and thrombin." Journal of Biomolecular Structure and Dynamics (2016) <http://dx.doi.org/10.1080/07391102.2016.1158665>
- ❖ **Akash Deep Biswas**, Sujata Dev, Mattaparthi Venkata Satish Kumar, "Characterization of the structure of *Anopheles gambiae* Odorant Receptor 1 (AgOR1) and its binding affinity with novel inhibitors and phytochemicals: A Molecular Dynamics and Docking Approach", International Journal of Innovations in Engineering and Technology, ISSN 2319-1058 <http://ijiet.com/wp-content/uploads/2016/05/84.pdf>

Under Review

- ❖ Vinod Kumar Yata, Varun Sharma, **Akash Deep Biswas**, Preetha Sundaram, Mattaparthi Venkata Satish Kumar. "Identification of *Cucumis stauvus* urease as a potential urea binding enzyme computational methods"

RESEARCH EXPERIENCE (2+ years)

Present

Designation: Doctoral Student
Institution: Scuola Normale Superiore, Pisa, Italy
Discipline: Methods and Models for Molecular Sciences
Duration: 19th December, 2016 to Present
Project: *In silico* infrared spectroscopy of complex systems

Past

Designation: Project Associate
Institution: Indian Institute of Technology, Kanpur, India
Department: Mechanical Engineering
Duration: 2nd February 2016 to November 2016
Project: Investigations into the thermo-oxidative stability and mechanical response of commercial polyimide resins and polyimide resin nano-composites for aerospace applications
Supervisors: Professor Sumit Basu & Dr. Nisanth N. Nair
Description: Developing MATLAB code for modelling Coarse Grain structures of high performance polymers and studying the mechanical behaviour of the same by applying the Molecular Dynamics Simulation technique using LAMMPS, locally developed scripts is being used for the visualization purpose

Past

Designation: Junior Research Fellow
Institution: Indian Institute of Technology, Guwahati, India
Department: Bioscience and Bioengineering
Duration: July 2015 to January 2016
Project: Structural and functional studies of translation initiation factors from *Pyrococcus horikoshii* OT3

Supervisor: Dr. Shankar Prasad Kanaujia

Description: To investigate the dynamic nature of metalloproteins by using Molecular Dynamics Simulation. GROMACS has been used to study the available 3D structures of 16 different proteins. Pymol has been used for visualization

Collaboration work during M.Sc. Thesis

Designation: M.Sc. Project Student

Institution: Tezpur University

Department: Molecular Biology and Biotechnology

Duration: January 2015 to June 2015

Project: An in silico approach to understand the structure-function properties of a serine protease (Bacifrinase) from *Bacillus cereus* and experimental evidence to support the interaction of Bacifrinase with fibrinogen and thrombin

Supervisors: Dr. Mattaparthi Venkata Satish Kumar & Professor Ashis K. Mukherjee

Description: For a correct formulation and commercialization of an enzyme, the detailed structure and functional study of the enzyme is very helpful. In this study, we focused on understanding the structure and ligand interaction of a protein purified from *Bacillus cereus* strain AB01 which was isolated from fermented food of North East India. The work has been published in Journal of Biomolecular Structure and Dynamics 2016

Collaboration work with NIT Jalandhar during M.Sc. Thesis

Designation: M.Sc. Project Student

Institution: Tezpur University

Department: Molecular Biology and Biotechnology

Duration: January 2015 to June 2015

Thesis: Identification of *Cucumis sativus* Urease as a potential urea binding enzyme by Computational Methods

Supervisors: Dr. Mattaparthi Venkata Satish Kumar & Dr. Vinod Kumar Yata

Description: Urea is a major component for plant growth and it is converted to Ammonia and Carbon dioxide by plant ureases. We have chosen *Pigeon pea* urease (PPU) as a reference for the binding site prediction as well to compare the extent of urea binding. We screened and selected *Cucumis sativus* urease (CSU) and *Fragaria vesca* urease (FVU) protein sequences for modelling. From the Molecular dynamics using AMBER and docking study using AutoDock we observed that our modelled structure of *Cucumis sativus* urease is equally stable and shows greater affinity towards urea than PPU.

EDUCATIONAL QUALIFICATION

Year of Passing	Degree	Institution/ Board	Grade/ Percentage
2015	Integrated M.Sc. in Bioscience and Bioinformatics (5 Years)	Tezpur University	6.94/10
2009	12 th	Kendriya Vidyalaya Khanapara, Guwahati	76.40%
2007	10 th	Kendriya Vidyalaya No. 1 Solmara, Tezpur	76.40%

ACADEMIC PROJECTS

M.Sc. Thesis (10th Semester)

Thesis: Characterization of the Structure of *Anopheles gambiae* Odorant Receptor 1(AgOR1) and its binding affinity with novel inhibitors: A Molecular Dynamics and Docking Approach

Institution: Tezpur University

Department: Molecular Biology and Biotechnology

Duration: January 2015 to June 2015

Supervisor: Dr. Mattaparthi Venkata Satish Kumar

Description: In a motive to design new drugs for the most affected and fatal disease malaria, we carried out the continuation work on *Anopheles gambiae* Odorant Receptor (AgOR1), we analysed the Docking results and took the best poses for further minimization and equilibration process. The trajectory files are used to study the Binding Free Energies using MM/PBSA-GBSA methods using AMBER

M.Sc. Thesis (9th Semester)

Thesis: Computational Study of Anopheles gambiae Odorant Receptor (AgOR1), A Molecular Dynamics and Molecular Docking Approach

Institution: Tezpur University

Department: Molecular Biology and Biotechnology

Duration: June 2014 to December 2014

Supervisor: Dr. Mattaparthi Venkata Satish Kumar

Description: *Anopheles gambiae* is responsible for Malaria spreading *Plasmodium falciparum*. The need of the hour is to get prominent and better repellents. To study the prominence order of few drugs we took an approach of molecular dynamics and molecular docking. The dynamics and interaction between *Anopheles gambiae* Odorant receptor (AgOR1) and Drugs are studied using AMBER

TECHNICAL AND SOFTWARE SKILLS

- ❖ Programming command in MATLAB, Fortran 95, Python 3
- ❖ Techniques known: Homology Modelling, Molecular Docking, Classical and Coarse Grain Molecular Dynamics Simulation, Free Energy Calculation
- ❖ Good command over AMBER, GROMACS, LAMMPS software for Molecular Dynamics Simulation
- ❖ Operating System: Windows 95/98/XP/Vista/7/8, LINUX
- ❖ Docking Tools: Molegro Virtual Docker, Auto Dock, Vina, Discovery Studio, Maestro – Schrödinger
- ❖ Other Tools: MATPLOTLIB, AurgusLab, ChemSketch, Chimera, Open Babel, Pymol, VMD, YASARA, Xmgrace, GNU plot etc.

RELEVANT COURSES

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|-----------------------------------------|------------------------------------------|
| ❖ Structural Bioinformatics | ❖ Bioinformatics software and Algorithms |
| ❖ Biological Database Management System | ❖ Biophysics |
| ❖ Bioprogramming | ❖ Computational Biology |
| ❖ Introductory Statistics | ❖ Basics in Bio-computing and IT |
| ❖ Mathematical Methods and PDE | ❖ Scientific Programming in Chemistry |
| ❖ Scientific Programming | ❖ Computational Spectroscopy |

INTERNSHIP

- ❖ Summer Intern at IIT Jodhpur from June-July, 2013 under the supervision of Dr. Ganesh Bagler

CONFERENCE, SEMINAR and Workshops

- ❖ Attended Workshop on “Computational Approaches to the Study of Protein Interaction, and Rational Drug Design” held by University of Padova, Italy
- ❖ Poster Presentation at National Conference on Recent Developments in Medicinal Biotechnology and Structure Based Drug Designing “*In silico* studies on a fibrin(ogen)olytic serine protease enzyme from *Bacillus cereus* AB01” held by Indian Institute of Technology, India
- ❖ Attended National Workshop on “QSAR/QSPR: Applications in Drug Designing” held in the Department of Molecular Biology and Biotechnology (MBBT), Tezpur University, India
- ❖ Poster Presentation at an Interactive Meet on Molecular Intricacies of Plant Pathogen Micro-organisms (MIPPM) “Identification of Effective Mosquito Repellents and checking its binding free energy from the extracts of *Ocimum tenuiflorum*” held by Tezpur University, India
- ❖ Attended National Workshop on “Exploring Biological Databases” held by Tezpur University, India
- ❖ Poster Presentation at International Conference on Disease Biology and Therapeutics, “Identification of Effective Mosquito Repellents from *Ocimum tenuiflorum* [TULASI PLANT]: A Computational Approach” held by Institute of Advanced Study in Science and Technology, India
- ❖ Poster Presentation at National Seminar on Recent Advances in Biotechnological Research in NorthEast India: Challenges and Prospects, “*In silico* Study: Effective Inhibitors for *Anopheles gambiae* Odorant Receptor (AgOR1)” held, Tezpur University, India

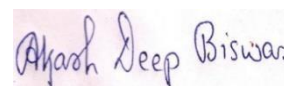
- ❖ Oral Presentation at lecture series on Recent Advances in Mathematical and Computational Biology, “Computational Study of *Anopheles gambiae* Odorant Receptor and its Repellents, A Molecular Dynamics and Docking Approach” held by NNMCB and Tezpur University, India
- ❖ Attended UGC-SAP National Seminar cum DBT-BIF Workshop on “Recent Advances in Microbial Bio-Technology and Molecular Evolution”, March 2013, Tezpur University, India
- ❖ Attended Workshop on Human Rights Awareness, 2011, Tezpur University, India
- ❖ Attended National Seminar on “Medicinal Plant and Microbe Diversity and their Pharmaceuticals” December 2010, Tezpur University, India

OTHER CURRICULAR ACTIVITIES

- ❖ Best Athlete Award of Tezpur University for Consecutive three sessions: 2011-12, 2012-13 & 2013-14
- ❖ Best Cadet Award (2nd Position) under the Group Headquarter Level, NCC for session 2013
- ❖ Secured National Rank 207th and State Rank 12th in C. V. Raman ‘Young Genius’ Award
- ❖ Interest: Cycling, Skating, Social running events
- ❖ Sports: Volley-Ball, Football, Swimming (KVS National Swimmer), Athletics

DECLARATION

I hereby declare that the information furnished above is true to the best of my knowledge and belief.



Akash Deep Biswas