Arghya Barman (Ph. D)
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Georgia State University
Department of Chemistry
Atlanta, GA 30302, USA

Objective

Challenging position in applying and developing computational chemistry and molecular simulation methods to understand biomolecular structure, function, and dynamics and develop molecular therapeutics for bio-medicinal applications.

Research Experiences

July 2013 – Present: Postdoctoral Associate, Department of Chemistry, Georgia State University
Advisor: Dr. Donald Hamelberg

Research Area: Exploring the dynamics and function of biomolecules and develop strategies for computer-aided-drug designing (CADD). Understanding the protonation behavior of active site residues in enzymes for their function using pKa shift calculations. Explore conformational space using free energy calculation to identify the toxic conformation of peptide. Develop and application of computational methodologies to capture the weak interactions in biomolecules. Understand the protein dynamics and identify the allosteric modulation of protein function to design alternative strategies for drug design. Finding the role of conserved water in structural stability of biomolecular function using free energy calculation. Involved in collaboration with cell biologist to identify novel molecules to alter enzyme function.

July 2012 – June 2013: Postdoctoral Fellow, Center for Biomolecular Therapeutics, University of Maryland Baltimore

Research Area: Support collaborative CADD projects. Implementation of MD simulations and *in silico* virtual screening to designing novel inhibitors for therapeutic targets.

Academic Achievements

Aug 2007- Jun 2012: Ph. D, Department of Chemistry, University of Miami, FL, USA.
Advisor: Dr. Rajeev Prabhakar.

Research Area: Understand the catalytic mechanism (bio-catalysts and organo-metallic catalysts) using MD simulation, QM and QM/MM. Mechanistic study of peptide aggregation and its role in ROS production through MD simulation and electronic structure calculation. Investigated the role of protonation state in inhibitor binding using molecular docking. Actively involved in several collaborative projects with synthetic chemist, biologist, physicist and medicinal chemists.

Thesis: "Mechanistic and structural studies of proteases, peptidases and amyloid beta peptide: an integrated computational approach"

Aug 2003-July 2005: M. Sc. (Biochemistry), Dept. of Biochemistry, University of Calcutta, India.
Advisor: Prof. Anjan K. Dasgupta

Project title: "High and low affinity ADP binding in P2Y receptors in human platelets and the role of the anti-stroke pro-drug Clopidogrel-A predictive *in silico* approach"

Jun 1999- May 2003: B. Sc. (Chemistry), University of Calcutta, India.

Employment

Oct 2005 – Jun 2007: Research Biologist, Chembiotek Research Intl. Pvt. Ltd (India)

Research Area: Protein purification (FPLC, Western blot, ELISA etc.), Cell culture (Sf9), Assay development (Radio and fluorophore based ligand binding assay)

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Expertise and Skills

Computational Chemistry

- MD Simulation of Bio-molecules to understand their dynamic behaviors.
- QM and QM/MM (ONIOM) calculations to optimize transition structures in catalytic pathways.
- Protein folding (Global and internal dynamics of peptides).
- Free energy calculations (Thermodynamic integration, umbrella sampling and PMF calculation)
- Calculation of reaction rates for enzyme catalysis.
- Homology modeling and loop modeling.
- Electrostatic calculations of biomolecules.
- Parameterization of small molecules using CGenFF.
- SILCS methodology for fragment based drug design.
- Molecular docking and virtual screening for ligand design and optimization.

Software and Programming

- Force filed: AMBER, CHARMM, OPLS and GROMOS.
- MD simulation package: AMBER, CHARMM and GROMACS.
- Electronic structure calculation: Gaussian03/09.
- Docking programs: Schrödinger Glide, AutoDock (Vina), DOCK and MOE.
- Scientific software: Originlab and Xmgrace.
- Electrostatic Calculation: Adaptive Posion Boltzmann Solver (APBS).
- Homology Modeling: MODELLER and Swiss Model.
- Visualization: Molden, Maestro, PyMol, VMD, YASARA and Rasmol.
- Programming language: Fortran77 and C++
- Scripting language: Shell script and Python.
- Linux operating system (Installing and maintaining hardware and software), Windows and Mac.

Awards

2012: South Florida ACS (SOFLACS) Graduate Travel Award.
2012: Max & Peggy Kriloff Student Travel Scholarship (University of Miami)
2011: Sam & Clara Schreiber Graduate Student Scholarship (University of Miami).
2005: Successful at all India GATE (Graduate Aptitude Test in Engineering) examination.

Poster and Oral presentations

2016: Poster Presentation (ACS 251st National Meeting, San Diego, CA)
"Conserved hydration site in Pin1 with unique water capturing motif".
2014: Oral Presentation (FAME 2014, Annual ACS meeting Florida, Innisbrook, FL)
"Cysteine mediated dynamic hydrogen bonding network in Pin1".
2012: Oral Presentation (ACS 243rd National Meeting, San Diego, CA)
"Insights into the substrate recognition and catalysis by β-secretase (BACE1) enzyme: A combined computational approach".
2011: Oral Presentation (FAME 2011, Annual ACS meeting Florida, Innisbrook, FL)
"Computational insights into substrate recognition and reactivity of ß-Secretase (BACE1) enzyme".
2010: Oral Presentation (FAME 2010, Annual ACS meeting Florida, Innisbrook, FL)
"Computational insights into the differential substrate recognition and catalysis by the ß-Secretase (BACE1) enzyme".
2009: Oral Presentation (FAME 2009, Annual ACS meeting Florida, Orlando, FL)
"Generation of Alzheimer's Amyloid β peptides (Aβ40 and Aβ42) by aspartyl protease activity of presenilin I".
2008: Poster presentation (FAME 2008, Annual ACS meeting Florida, Orlando, FL)
"Mechanism of metal catalyzed Methionine oxidation of Amyloid beta peptide".

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Invited Talks

1. Biomolecular simulations to probe molecular interactions and conformations in complex biological system. **(University of North Carolina, Chapel Hill, School of Pharmacy (2015))**
2. Cysteine mediated dynamic hydrogen bonding network in Pin1. **(FAME, Annual ACS meeting Florida, Innisbrook, FL (2014))**
3. Mechanistic and Structural Studies of Proteases, Peptidases and Amyloid beta Peptide: An Integrated Computational Approach. **(University of Maryland, Baltimorel, School of Pharmacy (2012)**

Professional Activities

Membership: American Chemical Society
Reviewer: Journal of Biomolecular Structure and Dynamics
Journal of Molecular Graphics and Modeling
Activities: Chaired sub session of Biochemistry section (FAME, 2014)
Judged Poster Session (FAME, 2014)
Judged Poster Session for MBD research fellows (GSU, 2015)

Teaching Experiences

- Taught freshman chemistry labs (CH113), an introductory course for under graduate students.
- Lab instructor for Physical chemistry lab (CHM364) for chemistry major students.
- Presented new material, designed and evaluated writing assignments, exams and grading.
- In person or group discussions to clarify concepts.
- Mentored and assisted undergraduate and graduate students in the field of theoretical and computational chemistry/biochemistry to accomplish research projects.
- Mentored NSF REU students and ACS project SEED students.

Publications:

1. Coupled dynamics and entropic contribution to allosteric mechanism of Pin1. **Arghya Barman** and Donald Hamelberg. Journal of Physical Chemistry B, 2016 DOI: 10.1021/acs.jpcb.6b02123 (***(IF: 3.302)***
2. Conserved hydration sites in Pin1 reveal a distinctive water recognition motif in protein. **Arghya Barman**, Crystal Lynn Smitherman, Michael Gregory Souffrant, Giovanni Gadda, and Donald Hamelberg, *Journal of Chemical Information and Modeling*, 2016, 56, 139-147 ***(IF: 3.738)***
3. Pushing the limits of the molecular mechanics force field to probe weak CH--π interactions in proteins. **Arghya Barman**, Bruce Batiste and Donald Hamelberg. *Journal of Chemical Theory and Computation.* 2015, 11, 1854-1863***(IF: 5.310)***
4. An Iron Reservoir to the Catalytic Metal: The Rubredoxin Iron in an Extradiol Dioxygenase. Fange Liu, Jiafeng Geng, Ryan H. Gumpper, **Arghya Barman**, Ian Davis, Andrew Ozarowski, Donald Hamelberg, and Aimin Liu, *Journal of Molecular Biology*, 2015, DOI:10.1074/jbc.M115.650259 ***(IF: 4.600)***
5. Loss of intra-molecular electrostatic interactions and limited conformational space may promote self-association of *cis*-tau peptide. **Arghya Barman** and Donald Hamelberg. *Proteins: Structure Function and Bioinformatics* 2015, 83,436-444. ***(IF: 2.921)***
6. Cysteine mediated dynamic hydrogen-bonding network in the active site of Pin1. **Arghya Barman** and Donald Hamelberg. *Biochemistry* 2014, 53, 3839-3850 ***(IF: 3.194)***
   (Theoretical prediction has been supported by experimental study: Biochemistry, 2015, DOI: 10.1021/acs.biochem.5b00606)

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7. Comparative molecular dynamics simulation studies for determining factors contributing to the thermostability of chemotaxis protein "CheY". Manish Paul, Mousumi Hazra, **Arghya Barman** and Saugata Hazra, *Journal of Biomolecular Structure and Dynamics*, 2014, 32, 928-949 ***(IF: 2.983)***
8. Catalytic mechanism of β-secretase enzyme in the presence of surrounding protein environment: A QM/MM study. **Arghya Barman** and Rajeev Prabhakar *Journal of Molecular Graphics and Modelling*. 2013, 40, 1-9. ***(IF: 2.022)***
9. Hydrocarbons Depending on the Chain Length and Head Group Adopt Different Conformations within a Water-Soluble Nanocapsule: 1H NMR and Molecular Dynamics Studies. Rajib Choudhury, **Arghya Barman**, Rajeev Prabhakar and V. Ramamurthy *Journal of Physical Chemistry B* 2013, 117, 398-407. ***(IF: 3.377)***
10. Protonation states of the catalytic dyad of β-secretase (BACE1) in presence of chemically diverse inhibitors: Insights from molecular docking study. **Arghya Barman** and Rajeev Prabhakar *Journal of Chemical Information and Modeling* 2012, 52 (5), 1275-1287. ***(IF: 4.068)***
11. Mechanism of Peptide Hydrolysis by Co-catalytic Metal Centers Containing Leucine Aminopeptidase Enzyme: A DFT Approach. Xiaoxia Zhu, **Arghya Barman**, Mehmet Ozbil, Tingting Zhang, Shanghao Li and Rajeev Prabhakar. *Journal of Biological Inorganic Chemistry* 2012, 17(2), 209-222. ***(IF: 3.164)***
12. Dimerization of the Full-Length Alzheimer's Amyloid β-Peptide (Aβ42) in Explicit Aqueous Solution: A molecular Dynamics Study. Xiaoxia Zhu, Ram Prasad Bora, **Arghya Barman**, Rajiv Singh and Rajeev Prabhakar *Journal of Physical Chemistry B* 2012, 116(15), 4405-4416. ***(IF: 3.377)***
13. Computational Modeling of Substrate Specificity and Catalysis of the β-secretase (BACE1) enzyme. **Arghya Barman**, Stephan Schürer, Rajeev Prabhakar. *Biochemistry* 2011, 50, 4337-4349. ***(IF: 3.194)***
14. Loss of cleavage at ß'-site contributes to the apparent increase of Aß secretion by BACE1-GPI processing of APP. Kulandaivelu S. Vetrivel, **Arghya Barman**, Ying Chen, Phuong D. Nguyen, Steven L. Wagner, Rajeev Prabhakar, and Gopal Thinakaran *Journal Biological Chemistry* 2011, 286, 26166-26177. ***(IF: 4.600)***
15. Cotinine modulates nicotinic receptors, reduces β-amyloid aggregation, and improves Alzheimer's pathology in mice. Valentina Echeverria, Ross Zeitlin, Sarah Burgess, **Arghya Barman**, Garima Thakur, Hideyo Inouye, Edmundo Feris, Magorzota Mamcarz, Li Wang, Steven D. Buckingham, Daniel A Kirschner, Takashi Mori, Roger M. Leblanc, Rajeev Prabhakar, David Sattelle, Roger L. Papke, and Gary W. Arendash. *Journal of Alzheimer's Disease* 2011, Volume 24, Number 4, 817-835. ***(IF: 3.612)***
16. Which One Among Aspartyl Protease, Metallopeptidase, and Artificial Metallopeptidase is the Most Efficient Catalyst in Peptide Hydrolysis? Ram P Bora, **Arghya Barman**, Xiaoxia Zhu, Mehmet Ozbil, Rajeev Prabhakar *Journal of Physical Chemistry B* 2010, 114, 10860–10875. ***(IF: 3.377)***
17. Insights into the Mechanism of Methionine Oxidation Catalyzed by Metal (Cu2+, Zn2+ and Fe3+) - Amyloid Beta (Aβ) Peptide Complexes: A Computational Study. **Arghya Barman**, Woody Taves, and Rajeev Prabhakar, *Journal of Computational Chemistry* 2009, 30(9), 1405-1413. ***(IF: 3.601)***
18. Computational Insights into Aspartyl Protease Activity of Presenilin 1 (PS1) Generating Alzheimer Amyloid β-Peptides (Aβ40 and Aβ42). Rajiv Singh, **Arghya Barman** and Rajeev Prabhakar *Journal of Physical Chemistry B* 2009, 113, 2990-2999. ***(IF: 3.377)***
19. Modeling the self-assembly dynamics of macromolecular protein aggregates underlying neurodegenerative disorders. Zhenyuan Zhao, Rajiv Singh, **Arghya Barman**, Neil F. Johnson, and Rajeev Prabhakar *Computational and Theoretical Nanoscience* 2009, 6(6), 1338-1351. ***(IF: 1.032)***

Reviews/Accounts/Perspectives:

1. Computational perspective and evaluation of plausible catalytic mechanisms of peptidyl-prolyl isomerases. Safia Tork Ladani, Michael Souffrant, **Arghya Barman** and Donald Hamelberg. *Biochimica et Biophysica Acta.* 2014. doi:10.1016/j.bbagen.2014.12.023. ***(IF: 3.829)***

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2. Theoretical Insights into the Functioning of Metallopeptidases and Their Synthetic Analogues. Tingting Zhang, Mehmet Ozbil, **Arghya Barman**, Thomas J. Paul, Ram Prasad Bora, and Rajeev Prabhakar. *Accounts of Chemical Research* 2015,48,192-200. ***(IF: 24.348)***
3. Computational Insights into Substrate and Site Specificities, Catalytic Mechanism and Protonation States of the Catalytic Asp Dyad of β-Secretase (BACE1). **Arghya Barman** and Rajeev Prabhakar. Scientifica, vol. 2014, Article ID 598728, 11 pages, 2014. doi:10.1155/2014/598728). ***(IF: 1.210)***
4. Computational Insights into Dynamics of Protein Aggregation and Enzyme−Substrate Interactions. Mehmet Ozbil, **Arghya Barman**, Ram Prasad Bora and Rajeev Prabhakar *Journal of Physical Chemistry Letter* ***(Perspective)*** 2012, 3, 3460−3469. ***(IF: 6.687)***