Abdullah Al Mamun
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SUMMARY OF QUALIFICATIONS

- PhD in Chemistry with over 8 years of hands-on experience in computational chemistry and biology focusing on drug discovery, human genomics, bioinformatics, molecular modeling, and computational method development
- Proficient in GPU-accelerated MD code, and skilled in quantum chemistry simulations for actionable drug discovery insights.
- Adept at collaborating with multidisciplinary teams, including ML experts, medicinal chemists, cell biologists, clinicians, geneticists, and software engineers, to advance multidisciplinary projects.
- Experienced in project management, leading multidisciplinary teams, and coordinating between internal and external stakeholders.
- Excellent communicator with a strong publication record, adept at translating complex scientific concepts into actionable strategies.

AREAS OF INTEREST

- Computational Chemistry and toxicology
- Protein and Enzyme design
- Small molecule drug discovery
- Human genomics
- Bioinformatics
- Computational method development
- Simulation and modeling
- Program management
- Data analysis and management

TECHNICAL SKILLS

- ***Methods:*** Molecular dynamics simulations, Monte Carlo simulation, ligand docking, homology modeling, enzyme design, Multiscale protein/ligand modeling (QM/MM), Quantum chemical calculations, Density Functional Theory (DFT), Time-dependent Density Functional Theory (TD-DFT), Parallel/HPC computing, Chromatography, GC-MS, GC, HPLC
- ***Machine learning codes:*** Alphafold, Rosettafold, ESMfold, Alphamissense, RF-diffusion, Protein-MPNN, Equibind
- ***Drug discovery codes:*** Rosetta, Schrodinger, MOE, BCL, Openbabel, Autodock
- ***Quantum Chemistry codes:*** Gaussian, Orca, Gamess-US
- ***Molecular Dynamics:*** Amber, Gromacs

- ***Visualization software:*** Pymol, MOE, VMD, Chimera, Gaussview, Chemcraft
- ***Plotting software and data analysis:*** Origin, Gnuplot, python
- ***Programming languages:*** C++, Python, and BASH scripting
- ***Operating systems:*** Linux, Windows and Mac
- ***Experimental techniques:*** GC-MS, HPLC, NMR

EDUCATION

Ph.D. in Chemistry **2020**
Department of Chemistry, University of Louisville, KY
M.S. Physical Chemistry **2018**
University of Louisville, Louisville, KY, USA
M.Sc. Inorganic Chemistry **2014**
University of Dhaka, Bangladesh
B.Sc. Chemistry **2013**
University of Dhaka, Bangladesh

WORK EXPERIENCES

Research Assistant Professor
Department of Chemistry, Vanderbilt University, Nashville, TN ***Jan. 2024 – present***

- Led computational chemistry and biology projects applying quantum, AI, and physics-based methods to support innovative drug discovery efforts.
- Applied computational chemistry and biology tools to investigate the genetic variance of individual patients in collaboration with an undiagnosed disease network at Vanderbilt University Medical Center.
- Applied computation method to improve variant effect prediction, pathogenecity prediction, gene annotation, and disease/phenotype- genotype alignment.
- Collaborated with a multi-disciplinary group to improve molecular models through AI and physics-based modeling.
- Applied computational chemistry and genomics tools to investigate the variants of unknown significance for patients with genetic disorders.
- Applied ligand-based QSAR model and structure-based virtual high throughput screening (vHTS) for HER2, ER-alpha, and PIK3CA candidate drugs.
- Mentored undergraduate, and graduate students as well as worked as a leader in a team of programmers, scientists, and graduate and undergraduate students.

Postdoctoral Research Scholar at Meilerlab,
Department of Chemistry, Vanderbilt University, Nashville, TN ***March 2020 – Dec. 2023***

- Applied conventional and enhanced molecular dynamics simulations (sMD, umbrella sampling, GaMD) to understand the effect of oncogenic mutations in different protein targets.

- Applied, Rosetta, Alchemical free energy method to calculate the binding affinity for different tyrosine kinase inhibitors both non-covalent and covalent.
- Applied QM/MM simulations to calculate the rate of activation for covalent inhibitors in HER2 protein target.
- Designed novel enzyme target using Rosetta ab initio enzyme design protocol and QM/MM method.
- Investigated the effect of oncogenic mutations in the juxtamembrane and transmembrane domain of Human epidermal growth factor receptor (EGFR) protein.
- Implemented a QM method in ROSETTA, to develop the ROSETTA QM method.

Graduate Research Assistant at Kozlowski's lab,
Department of Chemistry, University of Louisville, Louisville, KY. Jan. 2015- Feb. 2020

- Performed QM/MM simulation to understand the photochemical mechanism of AdoCbl-dependent ethanolamine ammonia lyase (EAL) and glutamate mutase (GLM) enzymes.
- Performed QM/MM and MD simulations to understand the photodissociation mechanism of AdoCbl in the biological photoreceptor CarH and MeCbl-dependent methionine synthase (MetH).
- Established a connection between photolysis and native catalysis in the activation of Co-C bond for AdoCbl-dependent enzymes using the QM/MM method.
- Performed QM/MM and MD and QM (DFT and ab initio) simulations to model the enzymatic reactions catalyzed by AdoCbl-dependent EAL and AdoCbl-dependent GLM.
- Elucidated the metal-centered and ligand-centered hydrogen evolution reaction (HER) using DFT.
- Performed DFT simulation for resonance Raman study of cobalamin cofactors.

AUTHORED PUBLICATIONS

1) **Mamun, A. A.,** Arnaldo Marin, Ariella Hanker, Jens Meiler, Carlos Arteaga; Enhancement of HER2/MAPK signaling and resistance to HER2 kinase inhibition by HER2 acquired mutations in HER2-mutant breast cancers; Cancer Research, 2022, DOI: 10.1158/0008-5472.CAN-22-3617.
2) Moth, C., **Mamun, A. A**., et al., VUStruct: a compute pipeline for high throughput and personalized structural biology, preprint, 2024, DOI: 10.1101/2024.08.06.606224
3) **Mamun A. A.,** Kim S., Zhang YK., Smith A., Lovely C., Brown B., Meiler J., Effects of transmembrane domain mutations in EGFR homo and heterodimerization, Manuscript in preparation
4) **Mamun A. A.,** Meiler J., Brown B. et. al., Random mutagenesis of NTRK gene fusions identifies recurrent gatekeeper and solvent front mutations that can be targeted with next generation TRK inhibitors, Manuscript in preparation.
5) B. Han, **Mamun A. A**., Gulsevin, A., Meiler J., Kenworthy, et. al., Design principles of Caveolins across metazoan and beyond, manuscript in preparation

6) Toda, M. J., Lodowski, P., **Mamun, A. A.** & Kozlowski, P. M. Photoproduct formation in coenzyme B12-dependent CarH via a singlet pathway, J. Photochem. Photobiol B, 232, 112471, 2022, https://www.sciencedirect.com/science/article/pii/S1011134422000859
7) Toda, M. J., Lodowski, P., **Mamun, A. A.** & Kozlowski, P. M. Electronic and photolytic properties of hydridocobalamin. J. Photochem. Photobiol. B 224, 112295 (2021), https://www.sciencedirect.com/science/article/pii/S1011134421001743.
8) Toda, M. J., **Mamun, A. A.,** Lodowski, P. & Kozlowski, P. M. Why is CarH photolytically active in comparison to other B12-dependent enzymes? J. Photochem. Photobiol. B 209, 111919, (2020), https://www.sciencedirect.com/science/article/pii/S1011134420303699.
9) Mieda-Higa, K., **Mamun, A. A.,** Ogura, T., Kitagawa, T. & Kozlowski, P. M. Resonance Raman investigation of dithionite-reduced cobalamin. J. Raman Spectrosc. 51, 1331–1342 (2020), https://onlinelibrary.wiley.com/doi/10.1002/jrs.5909. (Equal first author)
10) Toda, M. J., Lodowski, P., **Mamun, A. A.,** Jaworska, M. & Kozlowski, P. M. Photolytic properties of the biologically active forms of vitamin B12. Coord. Chem. Rev. 385, 20–43 (2019), https://www.sciencedirect.com/science/article/pii/S0010854518305484.
11) Cronin, S. P.**, Mamun, A. A.,** et al. Utilizing Charge Effects and Minimizing Intramolecular Proton Rearrangement to Improve the Overpotential of a Thiosemicarbazonato Zinc HER Catalyst. Inorg. Chem. 58, 12986–12997 (2019), https://doi.org/10.1021/acs.inorgchem.9b01912.
12) **Mamun, A. A.,** Toda, M. J., Lodowski, P. & Kozlowski, P. M. Photolytic Cleavage of Co–C Bond in Coenzyme B12-Dependent Glutamate Mutase. J. Phys. Chem. B 123, 2585–2598 (2019), https://doi.org/10.1021/acs.jpcb.8b07547.
13) **Mamun, A. A.,** Toda, M. J. & Kozlowski, P. M. Can photolysis of the CoC bond in coenzyme B12-dependent enzymes be used to mimic the native reaction? J. Photochem. Photobiol. B 191, 175–84 (2019), https://www.sciencedirect.com/science/article/pii/S1011134418312983.
14) Ghosh, A. P., **Mamun, A. A.** & Kozlowski, P. M. How does the mutation in the cap domain of methylcobalamin-dependent methionine synthase influence the photoactivation of the Co–C bond? Phys Chem Chem Phys 21, 20628–20640 (2019), http://dx.doi.org/10.1039/C9CP01849B.
15) Ghosh, A. P., **Mamun, A. A.,** Lodowski, P., Jaworska, M. & Kozlowski, P. M. Mechanism of the photo-induced activation of CoC bond in methylcobalamin-dependent methionine synthase. J. Photochem. Photobiol. B 189, 306–317 (2018), https://www.sciencedirect.com/science/article/pii/S1011134418309126.
16) Jain, R.**, Mamun, A. A.,** Buchanan, R. M., Kozlowski, P. M. & Grapperhaus, C. A. Ligand-Assisted Metal-Centered Electrocatalytic Hydrogen Evolution upon Reduction of a Bis(thiosemicarbazonato)Ni(II) Complex. Inorg. Chem. 57, 13486–13493 (2018), https://doi.org/10.1021/acs.inorgchem.8b02110.
17) **Mamun, A. A.,** Toda, M. J., Lodowski, P., Jaworska, M. & Kozlowski, P. M. Mechanism of Light-Induced Radical Pair Formation in Coenzyme B12-Dependent Ethanolamine Ammonia-Lyase. ACS Catal. 8, 7164–7178 (2018), https://doi.org/10.1021/acscatal.8b00120.
18) Islam, F., Majumder, S.S., **Mamun, A.A.,** Khan, M.B., Rahman, M.A., and Salam, A.; Trace metals concentrations at the atmosphere particulate matters in the Southeast Asian Mega City (Dhaka, Bangladesh). Open J. Air Pollut. 2015, 4, 86–98.

CONFERENCES & PRESENTATIONS

1) **Mamun A. A.,** Pawel M. Kozlowski, "Photochemistry of Adocobalamin-dependent ethanolamine ammonia-lyase" From Computational Biophysics to Systems Biology (CBSB), University of Cincinnati, May 2017 (Poster presentation)
2) **Mamun A. A.,** Pawel M. Kozlowski, "Photochemistry of Adocobalamin-dependent enzymes". 255th ACS National meeting, New Orleans, March 2018 (Poster presentation)
3) **Mamun A. A.,** Megan J. Toda, Pawel M. Kozlowski, "Mechanism of light-induced radical pair formation in AdoCbl-dependent glutamate mutase" ACS regional meeting, Augusta, Georgia, Oct 31-Nov 3, 2018 (Oral talk)
4) **Mamun A. A.,** Pawel M. Kozlowski, "Photodissociation mechanism of AdoCbl-dependent enzymes" GRADtalks Brown Bag Series, University of Louisville, November 2018 (Oral talk)
5) **Mamun A. A.,** Pawel M. Kozlowski, "Can photolysis of the Co-C bond be used to mimic the native enzymatic catalysis of the coenzyme B12?" Graduate Student Regional Research Conference (GSRRC), University of Louisville, February 27-28, 2019, (Oral Talk)
6) **Mamun A. A.,** Pawel M. Kozlowski, "Can photolysis of the Co-C bond in coenzyme B12-dependent enzymes be used to mimic the native enzymatic reactions". Biophysical Society Annual Meeting, Baltimore, Maryland, March 2-6, 2019 (Poster presentation)
7) **Mamun A. A.,** Pawel M. Kozlowski, "Connection between photolysis and native catalysis in AdoCbl-dependent enzymes" 51st Midwest Theoretical Chemistry Conference, June 6-8, 2019 (Poster presentation)
8) **Mamun A. A.,** Computational Modeling of Vitamin B12-Dependent Enzymatic Reactions: Mechanistic Insights, Vanderbilt University, September 21, 2019, (Invited talk)
9) Marin A. A., **Mamun A. A.,** et al., Abstract P4-01-02: A spectrum of secondary mutations in HER2 augment breast cancer cell growth and reduce neratinib sensitivity in HER2-mutant breast cancer, Cancer Res (2022) 82 (4_Supplement): P4-01-02, https://doi.org/10.1158/1538-7445.SABCS21-P4-01-02

AWARDS

- Doctoral Dissertation Completion Award, University of Louisville, Spring 2020
- Graduate Student Council Travel Award Spring 2019
- International Student Tuition Award, University of Louisville Fall 2018
- International Student Tuition Award, University of Louisville Spring- 2018
- The Graduate Network in Arts and Science (GNAS) Travel Award Spring- 2018