Amarda Shehu
Equity Champion

Professor
Computer Science Department
College of Engineering & Computing
George Mason University

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EMPLOYMENT

George Mason University

Associate Dean for AI Innovation, College of Engineering and Computing	July 2023 – present
Associate Vice President of Research for the Institute for Digital InnovAtion (idia.gmu.edu)	May 2022 – present

Co-Director of the Center of Excellence in Government Cybersecurity Risk Management and Resilience (crc.gmu.edu)
May 2023 – present

Inaugural Founding Co-Director of the Center for Advancing Human-Machine Partnerships (cahmp.gmu.edu), a George Mason University Provost Transdisciplinary Center for Advanced Study   August 2019 – May 2022

Professor, Department of Computer Science	August 2018 – present
Associate Professor, Department of Computer Science	August 2014 – August 2018
Assistant Professor, Department of Computer Science	August 2008 – 2014
Affiliate Appointment, School of Systems Biology	August 2008 – present
Affiliate Appointment, Department of Bioengineering	August 2011 – present

National Science Foundation

Program Director (IPA), Information Integration and Informatics	August 2019 – May 2022

Division of Information and Intelligent Systems, Directorate of Computer & Information Science and & Engineering

EDUCATION

Rice University, *Houston, TX*   December 2004 to July 2008
Ph.D. in Computer Science
Dissertation Title: *"Molecules in Motion: Computing Structural Flexibility"*
Committee: Kavraki LE (dissertation director), Vardi M, Clementi C, and Nakhleh L.

Rice University, *Houston, TX*   August 2002 to December 2004
M.S. in Computer Science
Thesis Title: *"Sampling Biomolecular Conformations with Spatial and Energetic Constraints"*
Committee: Kavraki LE (thesis director), Goldman R, Clementi C, and Nakhleh L.

Clarkson University, *Potsdam, NY*   January 2000 to May 2002
B.S. in Computer Science
Summa Cum Laude in two majors: (1) Computer Science and (2) Mathematics
Honor Thesis Title: *"Structural and Computational Complexity Results on Testing Dimension in Graphs"*
Honor Thesis Advisor: Tamon, C

SUMMARY OF ACCOMPLISHMENTS

Amarda is an internationally recognized researcher advancing foundational AI research that pushes the barriers of our understanding and addresses problems with societal resonance. She has a galvanizing and inclusive view of computing, as well as relentless energy and advocacy for computing research and scholarship for the advancement of knowledge across scientific disciplines and the improvement of the human condition. Amarda has published over 180 peer-reviewed research articles with postdoctoral, graduate, undergraduate, and high-school students.

Her passion for addressing complex/wicked real-world problems that bridge disciplines permeates her research, teaching, mentorship, and service. Her graduate and undergraduate courses integrate AI, Machine Learning, Robotics, Geometry, Statistical Mechanics, Physics, Biology, and Chemistry and attract and inspire diverse students in Computer Science, Electrical Engineering, Mathematics, Biophysics, Biology, Neuroscience, and Psychology.

Amarda's record shows a deep commitment to and championing of students of all backgrounds. Her professional activities expose a fierce advocate for diversity in the sciences with measurable impact in broadening the participation of historically-minoritized groups and turning struggle and hardship into stories of overcoming and success.

Amarda's leadership activities are driven by a firm commitment to bridging disciplines, breaking down silos, and cultivating an interdisciplinary, collaborative community to drive innovation across research, education, and workforce development programs in institutes of higher education. Since early 2024, Amarda represents Mason as lead PI on the Mason-NIST Artificial Intelligence Safety Institute Consortium cooperative research and development agreement (CRADA) within the Department of Commerce in response to Biden's Executive Order on Artificial Intelligence. She is becoming increasingly interested in the intersection of AI, Policy, and Regulation.

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[1] Text appearing in blue (darker in grayscale mode) is a hyperlink.

SELECTED AWARDS

† **Fellow of the American Institute for Medical and Biological Engineering (AIMBE), 2022**.

† **State Council of Higher Education of Virginia (SCHEV) Oustanding Faculty Award, 2022.**

† **National Science Foundation Director's Award for Superior Accomplishment (Group) as member of the NSF-wide Molecular Foundations for Biotechnology Program Working Group, 2022. Individual role: Representative of CISE.** .

† **National Science Foundation Director's Award for Superior Accomplishment (Group) as member of the NSF-wide COVID-19 RAPID Coordination Group, 2021. Individual role: Coordinator for CISE.**

† Editor's Choice, Best Paper, and Best Student Paper Awards, 2022, 2019, 2014, 2010.

† ACM Service Award in recognition of contributions to ACM-BCB, 2013.

† **NSF CAREER Award**, 2012.

† Honorable Mention, Humies Competition Award, ACM GECCO, 2012.

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† **George Mason University College of Engineering and Computing Faculty Excellence Award for Research**, 2024.

† **George Mason University Beck Family Presidential Medal for Faculty Excellence in Research and Scholarship**, 2021.

† **George Mason University Teaching Excellence Award**, 2018.

† **George Mason University Emerging Researcher/Scholar/Creator Award**, 2014.

† **George Mason University OSCAR Undergraduate Mentor Excellence Award**, 2013.

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† Outstanding Research Award, Department of Computer Science, GMU, 2022.

† Outstanding Research Award, Department of Computer Science, GMU, 2019.

† Outstanding Teaching Award, Department of Computer Science, GMU, 2018.

† Distinguished Service Award, Department of Statistics, GMU, 2017.

† Young Faculty Research Award, Department of Computer Science, GMU, 2012.

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† Recipient of 2007-2005 NIH Predoctoral Fellowship, Nanobiology Training Program.

† Clarkson University Presidential Scholarship, 2002-2000; Phi-Mu-Epsilon Fellowship Award for Best Clarkson University Student in Computer Science and Mathematics, 2001; Clarkson University Recognition Day Award, 2001; Hamlin/Darraugh Award and International Student Excellence Award 2001;

† Honorable mention at International Competition of Mathematics, Turkey, 1997; Winner of National Mathematics Olympiad, Albania, 1998-1994.

AVPR Highlighted Activities[2]

† Responsible for <u>Fuse</u> programming and activation, a new, first-in-the-region Public-Private-Partnership (P3) building central to Mason's re-envisioning of the Arlington Campus as Mason Square.

† Responsible for conceptualizing and implementing the <u>IDIA P3 Faculty Fellowship Program</u>, a new competitive award program that provides unlimited research support to Mason faculty. Purpose: Build IDIA identity and community, grow Mason's public-private partnership portfolio, and more closely align Mason R&D with the local, regional, and national industry.

† Responsible for conceptualizing and implementing the <u>IDIA Predoctoral Fellowship Program</u>, a new competitive award program that provides full award packages to predoctoral students across Mason. Purpose: Build IDIA identity and community, establish a predoctoral cohort model, and provide predoctoral students with agency to outline and work on emerging, transdisciplinary research problems and gather around themselves a team of faculty with the needed cross-disciplinary expertise.

† Responsible for conceptualizing and implementing the <u>IDIA CONNECT Series</u>, a series that brings leaders from industry, federal and local government, funding agencies, and non-profits to connect with faculty, researchers, and students on areas of mutural interest and complementarity. Purpose: grow public-private strategic partnerships.

† Responsible for conceptualizing and implementing the <u>IDIA AI Innovation Symposium</u>, a transdisciplinary symposium that brings faculty and researchers around organically-emerging AI-centric thematic areas. Purpose: identify interests, capabilities, and gaps on AI Innovation across Mason.

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[2]Serving in this capacity since May 2022. Only a few highlights of key activities that can be publicly-shared are listed.

† Responsible for identifying technologies of the future, bringing together units, leadership, and teams of faculty around such technologies, and outlining gaps, capabilities, and opportunities for strategic growth.

AD-CEC Highlighted Activities[3]

† Responsible for formulating an AI Roadmap and executing an AI Strategy for the College of Computing and Engineering along research, education, and workforce development.

† Responsible for conceptualizing and executing computing and engineering innovation activities that expand the footprint of the College (and more broadly the university) in unique problem spaces.

† Responsible for working with faculty and leading strategic, deliberate faculty teaming activities to expand the portfolio of the College in novel AI-centric or -supporting research and educational programs of value to our regional industry, funding agencies, including in the national defense and security space.

† Leading efforts in the College to revitalize and connect all College and Transdisciplinary Centers with partners, funders, faculty, and students and transform them into catalysts for innovation in the region and beyond.

† Supporting the Dean's office and working closely with other Associate Deans on faculty, graduate student, and undergraduate student affairs, including on TTIP pathways, timelines, and metrics.

† Working closely with the Divisional Dean of the School of Computing and the interim Division Dean of the School of Engineering on growing and creating new regional, national, and international partnerships.

† Aligning innovation activities and working closely with the Office of Diversity, Outreach, and Inclusive Learning in the College of Engineering and Computing to increase access for all students in the College.

NSF Program Director Highlighted Activities[4]

† Leader of NSF-Wide Working Group on Data Science Education and Training Program, 2022-2021. Role: Leading every aspect of the conceptualization-to-clearance process of new program.

† Leader of CISE-EHR Working Group on K9-12 Data Science Training Program, 2022-2021. Role: Leading every aspect of the conceptualization-to-clearance process of new DCL.

† Leader of NSF-wide Working Group on Harnessing Data Revolution: Data Science Corps Program, 2021-2019. Role: Led every aspect of the revision-to-clearance process of the 2021 HDR:DSC program. As leader of the 2nd round HDR:DSC competition, I also coordinated all the internal timelines, division of duties and panels among the PDs of the working group, award recommendations, budget yearly breakdowns, portfolio analysis, as well as reports and presentations to NSF leadership across the directorates involved. After the program concluded, I also coordinated with the communications office regarding advertising the program in NSF News and blogs.

† Member of NSF-wide working group on Molecular Foundations in Biotechnology Program, CISE Lead, 2022-2021. Role: Led CISE conceptualization and solicitation revision. Responsible for making AI a central methodological focus of the solicitation.

† CISE Liaison PD for NSF-Czech National Science Foundation (GACR) collaboration, 2021-2019. Role: Adjudication of requests on behalf of CISE.

† Member of NSF CISE-IIS Working Group on organizing initiatives to advance AI-Enabled Discovery, 2022-2020. Leading a \$1B AI-Enabled Discovery Big-Idea Pitch to CISE leadership (and AD).

† NSF representative Big Data Interagency Working Group across federal agencies, 2021-2019.

† Member of NSF-NIH Collaboration Working Group conceptualizing joint opportunities and programs, 2021-2019.

† Representative of NSF CISE directorate in NSF-wide Working Group and CISE Coordinator of NSF Coronavirus RAPID, 2020. Role: Adjudicated requests, identified relevant programs, tracked all steps of interest-to-award process, kept track of awards, and reported various data analysis aspects to CISE and NSF leadership.

† Conceptualized and galvanized the CISE research community and charged two prominent researchers, Jure Leskovec/Stanford and Marinka Zitnik/Harvard with organizing a two-day Symposium on novel therapeutics for COVID-19. I funded the symposium and assisted Jure and Marinka behind the scenes with recruiting diverse researchers and advertising in various scientific venues and student lists. The symposium attracted 1,840 participants from academia, industry, and non-profit, and the exchange of ideas and early results led to prominent interdisciplinary research on better understanding the proteomic profile of SARS-CoV2, as well as potential repurposed and novel therapeutics.

† Member of NSF-wide Traveling Working Group in AI & Nanobiology NSF Multiplier Mission for Czech Republic, CISE representative, 2020-2019. Role: evaluated "in-the-field" Czech capabilities in AI and Nanobiology and assisted together with PDs from EHR and MPS the OISE representative with the conceptualization and clearance of the NSF-GARC initiative that was approved by NSF and GACR leadership and went into effect in 2021.

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[3]Serving in this capacity since May 2023. Only a few highlights of key activities that can be publicly-shared are listed.
[4]2019-2022. What is shown here has been declassified and is shared with permission.

EXTERNAL FUNDING

26. NSF CISE Directorate: Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Conference Grant: "Large Language Models for Biological Discoveries (LLMs4Bio)," 03/01/2024 - 02/28/2025.
PIs: **Shehu A**; co-PIs: Bromberg Y/Emory University, Zhao L/Emory University.

25. Air Force Research Laboratory: "Digital Transformation Battle Lab," 11/15/2023 - 08/16/2024.
PIs: **Shehu A**, Josephson B, Archer G.

24. STTR Air Force: Topic No. AFX23E-TPCSO1-STTR Phase I - Proposal-FX23E-TPCSO1-0061 - "Metadata Overlay for Live-Streaming and Geolocating Security Incident Reporting System," 1/1/2024-3/31/2024.
PIs: Barbara D, **Shehu A**; Industrial partner: Pluribus [AF Contract: FA864924P008].

23. NSF CISE Directorate: Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Medium Collaborative Grant for "Learning Protein-ish: Foundational Insight on Protein Language Models for Better Understanding, Democratized Access, and Discovery," 08/01/2023 - 07/31/2026.
PI: **Shehu A**; co-PI: Bromberg Y/Emory University.

22. NSF BIO Directorate, Infrastructure Innovation for Biological Research (IIBR) Program Grant for "Collaborative Research: IIBR: Innovation: Bioinformatics: Linking Chemical and Biological Space: Deep Learning and Experimentation for Property-Controlled Molecule Generation," 08/01/2023 - 07/31/2026.
PI: **Shehu A**; co-PIs: Wuestl W and Zhang L/Emory University and Minbiole K/Villanova University

21. Commonwealth of Virginia Community Project Award for "Center of Excellence for Furthering U.S. Government Cybersecurity and IT Modernization Leadership and Governance," 09/01/2023 - 08/30/2024.
PI: **Shehu A**; co-PI: Auffret JP, Business/GMU.

20. CIA CHAOTICGOOD DTech Program for "Trustworthy Language Models," 01/01/2023 - 12/31/2023.
PI: Yao Z, CS/GMU; co-PIs: **Shehu A**; Liu M, CS/GMU.

19. U.S. Department of Defense MINERVA Research Initiative Award for "The cultural, economic, and institutional determinants of AI infrastructures and their consequences in global contexts," 07/01/2022 - 06/30/2025.
PI: Singh JP/GMU; co-PI: **Shehu A**; SP: Anastasopolous A/GMU; Kirkpatrick J/GMU; Hunzinger M/GMU.

18. Commonwealth of Virginia, Alzheimer's and Related Diseases Research Award for "Mechanisms of Amyloid Interaction and Signaling through the Nicotinic Receptor," 08/01/2019 - 06/39/2022.
PI: Kabbani N/GMU; co-PIs: **Shehu A**; Lucchini A/GMU.

17. NSF Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Small Grant for "Graph Generative Deep Learning for Protein Structure Prediction," 07/18/2018 - 07/31/2022.
PI: **Shehu A**; co-PI: Zhang L/GMU.

16. NSF Foundations of Emerging Technologies (FET): Collaborative Medium Grant for ""Automated Analysis and Exploration of High-dimensional and Multimodal Molecular Energy Landscapes," 07/26/2019 - 07/31/2023.
PIs: **Shehu A** and Plaku E/CUA; co-PI: Qiao W/GMU.

15. Jeffress Trust Awards Program in Interdisciplinary Research Award for "Modeling Protein Structure via Graph Generative Deep Learning," 06/30/2019 - 05/31/2020.
PI: Zhang L/IST-GMU; co-PI: **Shehu A**.

14. NSF Information and Intelligent Systems (IIS): Information Integration and Informatics (III): Collaborative Medium Grant for "Guiding Exploration of Protein Structure Spaces with Deep Learning," 07/01/2018 - 06/30/2021.
PIs: **Shehu A** and Chen J/UMissouri.

13. NSF Division of Mathematics Sciences (DMS) Grant for "Statistical Inference for Molecular Landscapes," 08/01/2018 - 07/31/2021.
PI: Qiao W/Statistics-GMU; co-PI: **Shehu A**.

12. Jeffress Trust Awards Program in Interdisciplinary Research Award for "High-dimensional Statistics and Biomolecular Modeling as a Powerful Microscope over Pathogenic Mutations in Proteinopathies," 06/15/2017 - 06/14/2018.
PI: Qiao W/Statistics-GMU; co-PI: **Shehu A**.

11. REU Supplement for NSF CCF Grant For "Novel Stochastic Optimization Algorithms for Advancing the Treatment of Dynamic Molecular Systems," 02/01/2017 - 06/30/2018.
PI: **Shehu A**; co-PI: De Jong, K.

10. REU Supplements for NSF CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 09/01/2016-02/01/2018.
PI: **Shehu A**, no co-PIs.

9. PFP/DARPA to PI: Stavrou A for "Enhanced Cyber Defense by Leveraging Involuntary Analog Emissions", Summer 2016.
Faculty Associate: **Shehu A**.

8. NSF Software Infrastructure for Sustained Innovation (Sustainable Software Elements – SSE) Collaborative Grant for "A Novel Plug-and-play Software Platform of Robotics-inspired Algorithms for Modeling Biomolecular Structures and Motions," 02/01/2015 - 01/31/2018.   PIs: **Shehu A**, Plaku E/CUA, Roitberg A/UF.

7. NSF Computing Core Foundations (CCF): Algorithmic Foundations (AF) Grant for "Novel Stochastic Optimization Algorithms for Advancing the Treatment of Dynamic Molecular Systems," 07/1/2014 - 06/30/2018.
PI: **Shehu A**; co-PI: De Jong, K.

6. NSF CISE Grant for "NSF CISE CAREER Writing Workshop," 12/05/2013 - 05/31/2014.   PI: **Shehu A**; co-PI: Rangwala H/Computer Science-GMU.

5. Jeffress Trust Awards Program in Interdisciplinary Research Award for "Probabilistic Search Algorithms: Powerful Novel Tools for Peptide Modeling," 09/15/2013 - 06/15/2015.
PI: **Shehu A**; co-PI: Blaisten-Barojas E/Computational Materials Science-GMU.

4. NSF REU Supplement for NSF CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 07/01/2013-06/30/2014.   PI: **Shehu A**, no co-PIs.

3. Virginia Foundation for Healthy Youth Award for "Molecular Mechanisms Underlying Menthol Cigarette Addiction," 07/01/2013 - 10/31/2015.   PI: Kabbani N/Neuroscience-GMU; co-PI: **Shehu A**.

2. NSF Information and Intelligent Systems (IIS): Robust Intelligence (RI) CAREER Grant for "Probabilistic Methods for Addressing Complexity and Constraints in Protein Systems," 03/01/2012 - 02/28/2017.
PI: **Shehu A**, no co-PIs.

1. NSF Computing Core Foundations (CCF): Algorithmic Foundations (AF) Grant for "A Unified Computational Framework to Enhance the Ab-initio Sampling of Native-like Protein Conformations," 9/1/2010 - 8/31/2014. PI: **Shehu A**, no co-PIs.

INTERNAL FUNDING

10. Curriculum Impact Grant for "Ethics and AI," Cross-Disciplinary Undergraduate Minor 06/01/2020-05-31/2022. PIs: **Shehu A**/CS-GMU, Jones R/PHI-GMU, Kirkpatrick J/PHI-GMU, Monea A/Cultural Studies-GMU, and Warweg P/CAHMP.

9. Provost's Transdisciplinary Center for Advanced Study Award for the "Center for Advancing Human-Machine Partnerships (CAHMP)," 08/25/2019-07-30/2024. PIs: **Shehu A**/CS-GMU, Lattanzi D/CEIE-GMU, and Bannan B/CEHD-GMU.

8. GMU Multidisciplinary Seed Funding Initiative in Modeling, Simulation, and Data Analytics for "An Integrative Multi-disciplinary Approach to Unravel and Target Viral Replication," 09/07/2017-05/31/2019).
PI: **Kehn-Hall K/SSB-GMU**, co-PIs: **Shehu A**/CS-GMU and Blaisten-Barojas E/CDS-GMU.

7. Mason Seed Grant for "Towards A Unified Dry to Wet Laboratory Framework for Screening, Modifying, and Designing Antimicrobial Peptides," 12/20/2013-05/01/2014.
PI: **Shehu A**, co-PI: Vidyashankar A/Statistics-GMU.

6. Mason Seed Grant for "Structural and Functional Mechanisms Underlying Menthol Addiction," 07/01/2013-10/01/2013.   PI: Kabbani N/Neuroscience-GMU, co-PI: **Shehu A**.

5. Mason Seed Grant for "Probabilistic Search Techniques as New Tools for Peptides Modeling," 12/01/2012-06/01/2013.   PI: **Shehu A**, co-PI: Cortes J/Robotics-University of Toulouse, France.

4. Mason Seed Grant for "Combining Experiment and Computation to Characterize Dopamine Receptors and the Mode of Action of Antipsychotic Drugs," 06/01/2010-06/01/2011.
PI: Kabbani N/Neuroscience-GMU, co-PI: **Shehu A**.

3. RA Support to Shehu, AY 2010-2011.

2. Bioengineering Seed Grant for "Staying Ahead of Evolution: Engineering Novel Antimicrobial Peptides," 01/01/2009-12/31/2010.   PI: **Shehu A**, co-PIs: Bishop B/Biochemistry-GMU and van Hoek M/Molecular Biology-GMU.

1. Mason Seed Grant for "In-silico Characterization and Design of Protein Complexes: Exploiting Symmetry and Redundancy," 01/01/2009-12/31/2009.   PI: **Shehu A**.

METRICS AT A GLANCE

As of June 2024: **3691** citations, h-index of **32**, i10-index of **89**

SELECTED REFEREED PUBLICATIONS

JOURNAL PUBLICATIONS[5]

J73. Lian Y[g], Bodian D, and **Shehu A***. *Elucidating the Role of Wildtype and Variant FGFR2 Structural Dynamics. Intl J Mol Sci* 25(8): 4523, 2024.

J72. Bromberg Y*, Kabir A[g], Ramakrishnan P, and **Shehu A***. *Variant Prediction in the Age of Machine Learning. Machine Learning and Protein Science*, Cold Spring Harbor Laboratory Press, 2023.

J71. Kabir A[g,*], Bhattarai M*, Rasmussen K, **Shehu A**, Usheva A, Bishop AR, and Alexandrov BS. *Dynamically Active Zone of DNA Breathing. Bioinformatics* 39(11):btad699, 2023. [IF: 5.8]

J70. Kabir A[g] and **Shehu A***. *GOProFormer: A Multi-Modal Transformer Method for Gene Ontology Protein Function Prediction. Biomolecules* 12(11):1709, 2022. [IF: 6.604]

J69. Qiao W* and **Shehu A**. *Space Partitioning and Regression Mode Seeking via a Mean-Shift-Inspired Algorithm. Electronic Journal of Statistics* 16(2):5623-5658, 2022. [IF: 1.125]

J68. Kabir KL[g], Ma B, Nussinov R, and **Shehu A***. *Fewer Dimensions, More Structures for Improved Discrete Models of Dynamics of Free versus Antigen-Bound Antibody. Biomolecules* 12(7):1011, 2022. [IF: 6.604]

J67. Alam FF[g] and **Shehu A***. *Data Size and Quality Matter: Generating Physically-realistic Distance Maps of Protein Tertiary Structures. Biomolecules* 12(7):908, 2022 (featured on issue cover), <u>*Editor's Choice 2022 Award.*</u> [IF: 6.604]

J66. Du Y[u], Guo X[g], **Shehu A**, and Zhao, L*. *Controlling the Generation of Molecules via Interpretable Variational Autoencoders. Bioinformatics* , btac296, 2022. [IF: 5.610]

J65. Kamranfar P[g], Lattanzi D Y*, **Shehu A***, and Stoffels S. *Pavement Distress Recognition via Wavelet-based Clustering of Smartphone Accelerometer Data. ASCE J of Computing in Civil Engineering*, 2021 (in press). [IF: 5.44]

J64. Guo X[g], Du Y[u], Tadepalli S[g], Zhao L, and Amarda Shehu**Shehu A***. *Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders. Bioinformatics Advances* 1:1(vbab036), 2021. [IF: 2.833]

J63. Zaman AB[g], Inan TT[g], De Jong KA, and **Shehu A***. *Adaptive Stochastic Optimization to Improve Protein Conformation Sampling. IEEE/ACM Trans Comput Biol and Bioinf (TCBB)*, 2021, online ahead of print (DOI: 10.1109/TCBB.2021.3134103). [IF: 3.015]

J62. Gogovi G[g], Silayi S[g], and **Shehu A***. *Computing the Structural Dynamics of RVFV L Protein Domain in Aqueous Glycerol Solutions. Biomolecules* 11(10):1427, 2021. [IF: 4.8797]

J61. Rahman T[g], Du Y[u], Zhao L, and **Shehu A***. *Generative Adversarial Learning of Protein Tertiary Structures. Molecules* 26(5):1209, 2021. [IF: 3.267]

J60. Akhter N[g], Kabir KL[g], Chennupati G, Vangara R, Alexandrov BS, Djidjev H, and **Shehu A***. *Improved Protein Decoy Selection via Non-Negative Matrix Factorization. IEEE/ACM Trans Comput Biol and Bioinf (TCBB)*, 2021, online ahead of print (DOI: 10.1109/TCBB.2020.3049088). [IF: 3.015]

J59. Alam FF[g] and **Shehu A***. *Unsupervised Multi-Instance Learning for Protein Structure Determination. J Bioinf and Comput Biol (JBCB)* 19(1):2140002, 2021. [IF: 1.063]

J58. Hoseini P[p], Zhao L, and **Shehu A***. *Generative Deep Learning for Macromolecular Structure and Dynamics. Curr Opin in Struct Biol*, Section on Theory and Simulation/Computational Methods 67: 170-177, 2021 (invited). [IF: 7.108]

J57. Bin Zaman A[g], Kamranfar P[g], Domeniconi C, and **Shehu A***. *Reducing Ensembles of Protein Tertiary Structures Generated De Novo via Clustering. Molecules* 25(9), 2228, 2020. [IF: 3.998]

J56. Tadepalli S[g], Barbara D, and **Shehu A***. *Anomaly Detection-based Recognition of Near-Native Protein Structures. IEEE Transactions on NanoBioscience* 19(3): 562-570, 2020. [IF: 1.955]

J55. Akhter N[g], Chennupati G, Djidjev H, and **Shehu A***. *Decoy Selection for Protein Structure Prediction Via Extreme Gradient Boosting and Ranking. BMC Bioinf* 21(Suppl 1):189,2020. [IF: 2.213]

J54. Alam FF[g], Rahman T[g], and **Shehu A***. *Evaluating Autoencoder-based Featurization and Supervised Learning for Protein Decoy Selection. Molecules* 25(5), 1146, 2020. [IF: 3.998]

J53. McDermott-Roe C*, Lu W, Maximova T[p], Wada S, Bukowy J, Marquez M, Lai S, **Shehu A**, Benjamin I, Geurts A, and Musunuru, K. *Investigation of a dilated cardiomyopathy–associated variant in BAG3 using genome-edited iPSC-derived cardiomyocytes. J of Clinical Investigation (JCI) Insight*, 4(22):e128799, 2019. [IF: 6.014]

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[5]Articles are listed in reverse chronological order. Shehu's advisees are indicated by (p) for postdoctoral, (g) for graduate, (u) for undergraduate, and (h) for high-school students. Corresponding authors are indicated by (*). Impact factors (IF) reported for journal publications are those at the year of publication. If not available, 5-year average or most recent values are reported. Acceptance Rates (AR) are reported for conference and workshop papers where available, whether obtained online or as reported in published proceedings.

J52. Kabir KL[g], Akhter N[g], and **Shehu A**[*]. *From Molecular Energy Landscapes to Equilibrium Dynamics via Landscape Analysis and Markov State Models. J Bioinf and Comp Biol* 17(6):1940014, 2019.   [IF: 0.845]

J51. Akhter N[g], Chennupati G, Kabir KL[g], Djidjev H, and **Shehu A**[*]. *Unsupervised and Supervised Learning over the Energy Landscape for Protein Decoy Selection. Biomolecules,* 9(1): 607, 2019.   [IF: 4.694]

J50. Zaman ABB[g] and **Shehu A**[*]. *Building Maps of Protein Structure Spaces in Template-free Protein Structure Prediction. J Bioinf and Comp Biol* 17(6):1940013, 2019.   [IF: 0.845]

J49. Zaman AB[g] and **Shehu A**[*]. *Balancing Multiple Objectives in Conformation Sampling to Control Decoy Diversity in Template-free Protein Structure Prediction. BMC Bioinf* 20, 211, 2019.   [IF: 2.511]

J48. Gogovi G[g], Almsned F[g], Ricci N[g], Kehn-Hall K, **Shehu A**, and Blaisten-Barojas E[*]. *Modeling the Tertiary Structure of the Rift Valley Fever Virus L protein. Molecules* 24(3), 781, 2019.   [IF: 3.060]

J47. Kabir KL[g], Hassan L[g], Rajabi[g], and **Shehu A**[*]. *Graph-based Community Detection for Decoy Selection in Template-free Protein Structure Prediction. Molecules* 24(3), 741, 2019.   [IF: 3.060]

J46. Nussinov R, Tsai C-J, **Shehu A**, and Jang, H. *Computational Structural Biology: The Challenges Ahead. Molecules* 24(3), 673, 2019.

J45. Morris D[g], Maximova T[p], Plaku E, and **Shehu A**[*]. *Attenuating Dependence on Structural Data in Computing Protein Energy Landscapes. BMC Bioinf* 20 (Suppl11), 280, 2019.   [IF: 2.511]

J44. Qiao W, Akhter N[g], Fang X[u], Maximova T[p], and **Shehu A**[*]. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes. BMC Genom* 19 (Suppl 7): 671, 2018.   [IF: 3.501]

J43. Akhter N[g], Qiao W, and **Shehu A**[*]. *An Energy Landscape Treatment of Decoy Selection in Template-free Protein Structure Prediction. Computation* 6(2):39, 2018 (invited to special issue on "Computation in Molecular Modeling").   [IF: 1.821]

J42. Veltri D, Kamath U, and **Shehu A**[*]. *Deep Learning Improves Antimicrobial Peptide Recognition. Bioinformatics* 34(16), 2740-2747, 2018.   [IF: 4.531]

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C3. Kamath U^g, De Jong KA*, and **Shehu A***. *Selecting Predictive Features for Recognition of Hypersensitive Sites of Regulatory Genomic Sequences with an Evolutionary Algorithm.* In Proc Genet and Evol Comp Conf (GECCO), Portland, Oregon, 2010, pg. 179-186.   [AR: 45%]

C2. Richardson SM, Olson B^g, Dymond JS, Burns S, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS*. *Automated Design of Assemblable, Modular, Synthetic Chromosomes.* In Proc Lecture Notes in Computer Science: Parallel Processing and Applied Mathematics (PPAM), 2009, vol. 6068, pg. 280-289.   [AR: 36%]

C1. **Shehu A***. *An Ab-initio Tree-based Exploration to Enhance Sampling of Low-energy Protein Conformations.* In Proc Robotics: Science and Systems (RSS), 2009, pg. 31-39.   [AR: 25%]

WORKSHOP PUBLICATIONS (PEER-REVIEWED)

W34. Inan TT^g, Liu M, and **Shehu A***. *Optimization Effectiveness versus Generalization Capability of Stochastic Optimization Algorithms for Deep Learning.* Intl Conf on Learning Representations (ICLR) 2024 Workshop on Bridging the Gap Between Practice and Theory in Deep Learning, Vienna, Austria, 2024.

W33. Moldwin A^g, Kabir A^g, and **Shehu A***. *A More Informative and Reproducible Remote Homology Evaluation for Protein Language Models.* LLMs4Bio Workshop at the 38th Annual AAAI Conference on Artificial Intelligence (AAAI), Vancouver, CA, 2024.

W32. Kabir A^g, Moldwin A, and **Shehu A***. *A Comparative Analysis of Transformer-based Protein Language Models for Remote Homology Prediction.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2022, pg. 1-8.

W31. Herceg M^{g*} and **Shehu A***. *Structure- and Energy-based Analysis of Small Molecule Ligand Binding to Steroid Nuclear Receptors.* In Proc Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2022, pg. 1-8.

W30. Rahman T^g, Alam FF^g and **Shehu A***. *Equivariant Encoding based GVAE (EqEn-GVAE) for Protein Tertiary Structure Generation.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W29. Wang Y^u, Ghaemi S^g, Ding A^u, Du Y^u, Pan B^g, Qin M^g, Lin X^g, Petersen AA^g, Leitgeb A^g, Alkhalifa S, Minbiole K, Wuest WM, Zhao L, and **Shehu A***. *Generation and Characterization of Quaternary Ammonium Compounds via Deep Learning.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W28. Pan B^g, Wang Y^u, Lin X^g, Qin M^g, Du Y^u, Ghaemi S^g, Ding A^u, Wang S^g, Alkhalifa S, Minbiole K, Wuest WM, Petersen AA^g, Leitgeb A^g, **Shehu A**, and Zhao L*. *Property-Controllable Generation of Quaternary Ammonium Compounds.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Las Vegas, Nevada, 2022, pg. 1-8.

W27. Pan B[g], Wang Y[u], Lin X[g], Du Y[u], Ghaemi S[g], Ding A[u], Wang S[g], **Shehu A**, and Zhao L[*]. *Property-Controllable Generation of Quaternary Ammonium Compounds.* In Proc ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) Workshop on Deep Learning on Graphs: Methods and Applications (DLG-KDD'22), Washington, D.C., 2022.

W26. Kamranfar P[g], Lattanzi D, **Shehu A**, and Barbara D[*]. *Multiple Instance Learning for Detecting Anomalies over Sequential Real-World Datasets.* In Proc ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD) Workshop on Anomaly and Novelty Detection (ANDEA) , Washington, D.C., 2022.

W25. Du Y[u], Guo X, **Shehu A**, and Zhao L[*]. *Interpretable Molecular Graph Generation via Monotonic Constraints.* In Proc Neural Information Processing Systems (NeurIPS) Workshops: ML4Molecules, Virtual, 2021.

W24. Alam FF[g] and **Shehu A**[*]. *Generating Physically-Realistic Tertiary Protein Structures with Deep Latent Variable Models Learning Over Experimentally-available Structures.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Virtual, 2021, pg. 1-8.

W23. Kabir KL[g], Ma B, Nussinov R, and **Shehu A**[*]. *Antigen Binding Reshapes Antibody Energy Landscape and Conformation Dynamics.* In Proc IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM) Workshops: Computational Structural Biology Workshop (CSBW), Virtual, 2021, pg. 1-8.

W22. Du Y[u], Guo X[g], Zhao L[*], and **Shehu A**[*]. *Interpretable Molecule Generation via Disentanglement Learning.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2020, pg. 1-8.

W21. Du Y[u], Kabir A[g], Zhao L[*], and **Shehu A**[*]. *From Interatomic Distances to Protein Tertiary Structures with a Deep Convolutional Neural Network.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, 2020, pg. 1-8.

W20. Zaman AB[g], Kamranfar P[g], Domeniconi C, and **Shehu A**[*]. *Decoy Ensemble Reduction in Template-free Protein Structure Prediction.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Buffalo, NY 2019, pg. 562-567.

W19. Alam FF[g], Rahman [g], and **Shehu A**[*]. *Learning Reduced Latent Representations of Protein Structure Data.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Buffalo, NY 2019, pg. 592-597.

W18. Dua M[g], Veltri D, Bishop B, and **Shehu A**[*]. *Guiding Exploration of Antimicrobial Peptide Space with a Deep Neural Network.* IEEE BIBM Workshops: Artificial Intelligence Techniques for BioMedicine and HealthCare (AIBH), Madrid, Spain 2018, pg. 2082-2087.

W17. Hassan L[g], Rajabi Z[g], Akhter N[g], and **Shehu A**[*]. *Community Detection for Decoy Selection in Template-free Protein Structure Prediction.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D.C. 2018, pg. 621-625.

W16. Almsned F[g], Gogovi G[g], Bracci[g], Kehn-Hall K, Blaisten-Barojas E, and **Shehu A**[*]. *Modeling the Tertiary Structure of a Multi-domain Protein.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D.C. 2018, pg. 615-620.

W15. Sapin E[p], De Jong KA, and **Shehu A**[*]. *Evolving Conformation Paths to Model Protein Structural Transitions.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Boston, MA, 2017, pg. 673-678.

W14. Qiao W[*], Maximova T[p], Plaku E, and **Shehu A**[*]. *Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Boston, MA, 2017, pg. 679-684.

W13. Sapin K[p], De Jong KA, and **Shehu A**[*]. *An Evolutionary Algorithm to Model Structural Excursions of a Protein.* In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Berlin, Germany, 2017, pg. 1669-1673.

W12. Sapin K[p], De Jong KA, and **Shehu A**[*]. *Path-based Guidance of an Evolutionary Algorithm in Mapping a Fitness Landscape and its Connectivity.* In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Denver, CO, 2016, pg. 1293-1298.

W11. Sapin K[p], De Jong KA, and **Shehu A**[*]. *Mapping Multiple Minima in Protein Energy Landscapes with Evolutionary Algorithms.* In Workshop on Evolutionary Algorithms for Computational Structural Biology - Genet and Evol Comp Conf (GECCO) Workshops, Madrid, Spain, 2015, pg. 923-927.

W10. Molloy K[g], Clausen R[g], and **Shehu A**[*]. *On the Stochastic Roadmap to Model Functionally-related Structural Transitions in Wildtype and Variant Proteins.* In Workshop on Robotics Methods for Structural and Dynamic Modeling of Molecular Systems - Robotics: Science and Systems (RSS) Workshops, Berkeley, CA, 2014, pg. 1-6.

W9. **Shehu A**[*] and De Jong KA. *Memetic, Multi-Objective, Off-Lattice, and Multiscale Evolutionary Algorithms for De-novo and Guided Protein Structure Modeling.* In Workshop on Natural Computing for Protein Structure Prediction - Intl Conf on Parallel Problem Solving from nature (PPSN) Workshops, Ljubljana, Slovenia, 2014, pg. 1-2.

W8. Clausen R^g and **Shehu A***. *Exploring the Structure Space of Wildtype Ras Guided by Experimental Data.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 757-764.

W7. Hashmi I^g and **Shehu A***. *Informatics-driven Protein-protein Docking.* In Comput Struct Biol Workshop (CSBW) - ACM BCB Workshops, Washington, D. C., 2013, pg. 772-779.

W6. Olson B^g and **Shehu A***. *An Evolutionary Search Algorithm to Guide Stochastic Search for Near-native Protein Conformations with Multiobjective Analysis.* In Workshop on Artificial Intelligence and Robotics Methods in Computational Biology - Intl Conf of Association for Advancement of Artificial Intelligence (AAAI) Workshop, Bellevue, WA, 2013, pg. 32-37.

W5. Molloy M^g and **Shehu A***. *A Robotics-inspired Method to Sample Conformational Paths Connecting Known Functionally-relevant Structures in Protein Systems.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 56-63. [AR: 33%]

W4. Saleh S^u, Olson B^g, and **Shehu A***. *A Population-based Evolutionary Algorithm for Sampling Minima in the Protein Energy Surface.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Philadelphia, PA, 2012, pg. 48-55. [AR: 33%]

W3. Olson B^g, Hendi, S-F^g, and **Shehu A***. *Protein Conformational Search with Geometric Projections.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 366-373. [AR: 40%]

W2. Akbal B, Hashmi I^g, **Shehu A**, and Haspel N*. *Refinement of Docked Protein Complex Structures Using Evolutionary Traces.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 400-404. [AR: 40%]

W1. Hashmi I^g, Akbal B, Haspel N, and **Shehu A***. *Protein Docking with Information on Evolutionary Conserved Interfaces.* In Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshops, Atlanta, GA, 2011, pg. 358-365. [AR: 40%]

BOOK CHAPTERS (PEER-REVIEWED)

B7. Kabir A^g and **Shehu A***. *Graph Neural Networks for Predicting Protein Function, Activity, and Molecular Interactions.* In Graph Neural Networks on Proteins and DNA. Springer Series on Graph Neural Networks: Foundations, Frontiers, and Applications, first edition, (Editors: Wu, L., Cui, P., Pei, J., and Zhao, L.), 2021.

B6. Akhter N^g, Hassan L^g, Rajabi Z^g, Barbará D, and **Shehu A***. *Learning Organizations of Protein Energy Landscapes: An Application on Decoy Selection in Template-Free Protein Structure Prediction.* In Methods in Molecular Biology: Protein Supersecondary Structure (Springer), first edition, (Editor: Kister, A.), 2018.

B5. Kamath U, Domeniconi C, **Shehu A**, and Kenneth De Jong*. *EML: A Scalable, Transparent Meta-Learning Paradigm for Big Data Applications.* In Intelligent Systems Reference Library: Innovations in Big Data Mining and Embedded Knowledge (Springer), first edition, (Editor: Anna Esposito, Antonietta M. Esposito, and Lakhmi C. Jain), 2018.

B4. **Shehu A***, Barbará D, and Molloy K. *A Survey of Computational Methods for Protein Function Prediction.* In Big Data Analytics in Genomics (Springer), first edition, (Editors: Wong, KC), 2016.

B3. **Shehu A** *A Review of Evolutionary Algorithms for Computing Functional Conformations of Protein Molecules.* In Computer-Aided Drug Discovery (Springer Methods in Pharmacology and Toxicology Series), first edition, (Editors: Zhang W), 2015.

B2. **Shehu A** *Probabilistic Search and Optimization for Protein Energy Landscapes.* In Handbook of Computational Molecular Biology, Chapman & Hall/CRC Computer & Information Series, 2nd edition (Editors: Aluru S and Singh M), 2013.

B1. **Shehu A**. *Conformational Search for the Protein Native State.* In Protein Structure Prediction: Method and Algorithms, Wiley Book Series on Bioinformatics, 2009.

ABSTRACTS, POSTERS, AND EXTENDED ABSTRACTS[6]

A75. Peterson AA^g, Leitgeb A^g, Alkhalifa S, Zhao L, **Shehu A**, Wuest WM, and Minbiole K*. *Incorporation of Machine Learning Strategies in the Development of Quaternary Ammonium Compounds.* American Chemical Society National Meeting, Indianapolis, IN, March, 2023.

A74. Herceg M^g, Brown M, and **Shehu A***. *Computational evidence of BRCA1-NC3 receptor interaction and druggability analysis in BRCA1-related oncogenesis.* American Society of Human Genetics Symposium, Virtual, October, 2021 (Poster).

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[6]Abstracts are typically 1-2 paragraph submissions that are lightly reviewed and accepted either as poster or oral presentations at conferences and workshops; in the case of oral presentations, such as at 3DSIG, the review process is more rigorous. Extended abstracts are typically viewed as condensed manuscript submissions of 1-3 pages and are also more rigorously reviewed. All extended abstracts listed in this CV are indexed by ACM or IEEE and assigned their own doi.

A73. Liang Y[g], Bodian D, and **Shehu A**[*]. *3D conformation analysis of the FGFR2 kinase domain with disease-associated mutations reveals novel features that correlate with clinical presentation.* American Society of Human Genetics Symposium, Virtual, October, 2021 (Poster).

A72. Dua M[g], Veltri D, Bishop B, and **Shehu A**[*]. *Exploring the Space of Antimicrobial Peptides Guided by a Deep Learning Model.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

A71. Kabir, LK[g], Akhter N[g] and **Shehu A**[*]. *Unsupervised Learning of Conformational States Present in Molecular Dynamics Simulation Data for Summarization of Equilibrium Conformational Dynamics.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

A70. Akhter N[g] and **Shehu A**[*]. *Unsupervised Learning for Decoy Selection in Protein Structure Prediction.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

A69. Zaman AB[g] and **Shehu A**[*]. *A Multi-Objective Stochastic Optimization Approach for Decoy Generation in Template-Free Protein Structure Prediction.* Biophysical Society Meeting, Baltimore, MD, March, 2019 (Poster).

A68. Roychoudhoury S[h] and **Shehu A**[*]. *Systematic Study of Different Design Decisions in Markov Model-based Analysis of Molecular Structure Data.* (extended abstract and poster presentation, pg. 508-509). ACM BCB. Washington, DC, August 29 - September 01, 2018. (*Honorable Mention*)

A67 Molloy K, Akhter N[g], and **Shehu A**[*]. ACM-BCB '18 Tutorial: *Modeling Macromolecular Structures and Motions: Computational Methods for Sampling and Analysis of Energy Landscapes.* (abstract and tutorial presentation, pg. 554). ACM BCB. Washington, DC, August 29 - September 01, 2018.

A66. **Shehu A**[*]. *Reconstruction and Mining of Energy Landscapes of Ras Variants.* Ras Initiative Symposium. Frederick National Laboratory for Cancer Research, National Cancer Institute, Frederick, MD, December 6-8, 2017. (Abstract and Poster).

A65. **Shehu A**[*]. *Guiding Stochastic Optimization Algorithms with Experimental Data to Model Protein Energy landscapes and Structural Transitions.* Thematic Meeting of the Biophysical Society: Conformational Ensembles from Experimental Data and Computer Simulations. Berlin, Germany, August 25-29, 2017. (Abstract and Poster).

A64. Molloy K, Morris D[g], and **Shehu A**[*]. "ACM-BCB '17 Tutorial: *Robotics-inspired Algorithms for Modeling Protein Structures and Motions.* (abstract and tutorial presentation, pg. 628). ACM BCB. Boston, MA, August 20-23, 2017.

A63. Maximova T[p], Qiao W, Plaku E, Plaku E, Mattos C, Ma B, Nussinov R, and **Shehu A**[*]. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes.* 3DSIG at Intelligent Systems for Molecular Biology (ISMB). Prague, Czech Republic, July 22-23, 2017. (Abstract and Oral Presentation).

A62. Sapin E[p], De Jong KA, and **Shehu A**[*]. *Evolutionary Search for Paths on Protein Energy Landscapes.* ACM GECCO, Berlin, Germany, July 15-19, 2017. (Two-page poster paper).

A61. **Shehu A**[*]. *Big, Molecular Structure Data Demand Automated Landscape Analysis.* UC Davis RTG Statistical Sciences Symposium: Geometry, Statistics, and Data Analysis. Davis, California, May 19-20, 2017. (Poster and Abstract).

A60. Maximova T[p], Plaku E, and **Shehu A**[*]. *Method for Extended Sampling and Transition Paths Prediction with Probabilistic Roadmap Algorithm.* 3DSig, Intelligent Systems for Molecular Biology (ISMB) Orlando, Florida, July 2016 (Poster and Extended Abstract). <u>*Outstanding Research Presentation Award*</u>).

A59. Marquez M, McDermott-Roe C[*], Bukowy J, Kolander K, Kuo J, Maximova T[p], **Shehu A**, Benjamin I, and Geurts A. *Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.* Keystone Symposia on Molecular and Cellular Biology: Heart Failure: Genetics, Genomics and Epigenetics, Snowbird Resort, Snowbird, Utah, April 2016 (Poster and Abstract).

A58. McDermott-Roe C[*], Mitzefelt K, Marquez M, Grzybowski M, Bukowy J, Maximova T[p], **Shehu A**, Benjamin I, and Geurts A. *Modeling BAG3-associated cardiomyocyte dysfunction via genome editing in induced pluripotent stem cells.* CRISPR Precision Gene Editing Congress, Boston, Massachussetts, February 2016 (Poster and Abstract).

A57. Mazyar K[u], Hashmi I[g], Neil A, and **Shehu A**[*]. *Platform to Support Intensive Webserver Computations on Argo.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).

A56. Songyue H[u] and **Shehu A**[*]. *A new Distance Function for Protein Structures for the Decoy Selection Problem in De-novo Structure Prediction.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration, Fairfax, VA, April 2015 (Poster).

A55. Clausen R[g], **Shehu A**[*], Ma B, and Nussinov R. *A Novel Evolutionary Algorithm to Model Energy Landscapes of Wildtype and Variant Sequences of H-Ras.* Biophysical Society Meeting, Baltimore, MD, February, 2015 (Poster).

A54. Clausen R[g], **Shehu A**[*], Ma B, and Nussinov R. *Mapping the Structure Space of the Ras Protein using a Novel Hybrid Evolutionary Algorithm.* NIH Summer Poster Day, Fredericks, MD, July, 2014 (Poster).

A53. Van MJ[u], Namazi M[u], Xiang R[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *Structural Analysis and Dynamics of the Met-Enkephalin Peptide.* American Chemical Society (ACS) Undergraduate Research Poster Session, Charlottesville, VA, April 2014 (Poster).

A52. Pilapitiya H[u], Kabbani N[*], and **Shehu A**[*]. *Modeling Binding of Amyloid beta-42 Peptide to the Alpha 7 Nicotinic Receptor.* Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

A51. Van MJ[u], Namazi M[u], Xiang R[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *Conformational Sampling and Principal Component Analysis of the Met-Enkephalin Peptide.*Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

A50. Namazi M[u], Van MJR[u], Xiang R[u], **Shehu A**[*] and Blaisten-Barojas E[*]. *Molecular Dynamics Simulation of the Met-Enkephalin Peptide with Explicit Solvent.*Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

A49. Xiang R[u], Van MJR[u], Namazi M[u], Blaisten-Barojas E[*], and **Shehu A**[*]. *A Clustering Algorithm for Molecular Structures: Application on the Met-Enkephalin Peptide.*Mason Annual Volgenau School of Engineering Undergraduate Research Celebration and the Mason COS Undergraduate Research Colloquium, Fairfax, VA, April 2014 (Poster).

A48. Clausen R[g] and **Shehu A**[*]. *A PCA-guided Search Algorithm to Probe the Conformational Space of the Ras Protein.* ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).

A47. Hashmi I[g] and **Shehu A**[*]. *Protein-protein Docking using Information from Native Interaction Sites.* ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C., September 2013 (Extended Abstract and Poster).

A46. Olson B[g] and **Shehu A**[*]. *A Multi-objective Guided Evolutionary Search Algorithm for Sampling Near-native Protein Conformations.* Workshop on Artificial Intelligence and Robotics Methods for Computational Biology - Conf on Association for Advancement of Artificial Intelligence Workshop, Bellevue, WA, July 2013 (Poster).

A45. Randou EG, Veltri D[g], and **Shehu A**[*]. *Towards Classification and Virtual Screening of Antimicrobial Peptides with Regression-based Binary Response Models.* Nonclinical Biostatistics Conference (NCB), Villanova University, PA, 2013 (Abstract and Oral Presentation).

A44. Molloy K[g], Van JM[u], Barbara D, and **Shehu A**[*]. *Higher-order Representations for Automated Organization of Protein Structure Space.* Celebration of Undergraduate Student Scholarship, George Mason University, Fairfax, VA, May 2013 (Poster).

A43. Saleh S[u], Olson B[g], and **Shehu A**[*]. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* National Council of Undergraduate Research (NCUR), University of Wisconsin-La Crosse, La Crosse, WI, 2013 (Abstract and Poster).

A42. Shehu A. *Probabilistic Methods for Modeling Structures and Motions of Protein Systems.* NFS Grants Conference, Fairfax, VA, 2012 (Poster).

A41. Bohidar N[h] and **Shehu A**[*]. *From Coarse-grained Conformations to Motion Pathways in Proteins.* Thomas Jefferson Senior Research Day, Alexandria, Virginia, April 2013 (Poster).

A40. Reinstadler B[u], Van JM[g], and **Shehu A**[*]. *Supersecondary Structure Motifs and De Novo Protein Structure Prediction.*Grace Hopper Conference Celebration of Women in Computing, Baltimore, MD, 2012 (Abstract and Poster).

A39. Saleh S[u], Olson B[u] and **Shehu A**[*]. *An evolutionary framework to sample near-native protein conformations.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 933. (Extended Abstract and Poster).

A38. Veltri D[*] and **Shehu A**[*]. *Physico-chemical features for recognition of antimicrobial peptides.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 942. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

A37. Olson B[g] and **Shehu A**[*]. *An evolutionary search framework to efficiently sample local minima in the protein conformational space.* ACM BCB, pg. 590. Orlando, FL, 2012 (Extended Abstract and Poster).

A36. Hashmi I[g] and **Shehu A**[*]. *Sampling low-energy protein-protein configurations with basin hopping.* IEEE BIBM, pg. 947. Philadelphia, PA, October 4-7, 2012. (Extended Abstract and Poster, *Best Poster Award*).

A35. Olson B^g and **Shehu A***. *Jumping low, jumping high: Controlling hopping in the protein energy surface.* IEEE BIBM, pg. 946. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

A34. Molloy K^g and **Shehu A***. *A tree-based search to bias sampling of protein decoy conformations.* IEEE BIBM, pg. 978. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

A33. Molloy K^g and **Shehu A***. *Mapping conformational pathways between known functional protein states.* CSBW at IEEE BIBM Workshops (BIBM-W), pg. 971. Philadelphia, PA, October 4-7, 2012 (Extended Abstract and Poster).

A32. Jordan S^u and **Shehu A***. *Refinement of Coarse-grained Near-native Protein Conformations Using AMBER FF99SB Force Field.* Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, Summer 2012 (Poster).

A31. Saleh S^u, Olson B^g, and **Shehu A***. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* Celebration of Student Scholarship, Fairfax, VA, May 2012 (Poster).

A30. Saleh S^u, Olson B^g, and **Shehu A***. *Revisiting Evolutionary Search for Effective Sampling of Near-native Conformations in the Protein Conformational Space.* Virginia Academy of Sciences, Norfolk, VA, May 2012 (Abstract and Poster).

A29. Saleh S^u and **Shehu A***. *An Evolutionary-inspired Probabilistic Search Algorithm to Structurally Characterize the Native State of a Novel Protein Sequence.* College of Science Symposium, George Mason University, Fairfax, VA, May 2012 (Poster).

A28. Olson B^g and **Shehu A***. *A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.* 26th Annual Meeting of the Protein Society, San Diego, CA, 2012 (Abstract and Poster).

A27. Olson B^g and **Shehu A***. *A Basin Hopping Probabilistic Search Framework to Efficiently Sample Local Minima in the Protein Conformational Space.* Intelligent Systems for Molecular Biology (ISMB) Student Council, Long Beach, CA, 2012 (Abstract and Poster).

A26. Molloy K^g and **Shehu A***. *Assembly of Low-Energy Protein Conformations with Heterogeneous Fragments.* IEEE BIBM, pg. 991-993. Atlanta, GA, November 12-15, 2012 (Extended Abstract and Poster).

A25. Olson B^g and **Shehu A***. *Mapping the Protein Conformational Landscape with Adaptive Probabilistic Search.* 55th Annual Meeting of the Biophysical Society, Baltimore, Maryland, 2011 (Abstract and Poster).

A24 : Hashmi I*, Akbal-Delibas B, Haspel N, and **Shehu, A***. *Protein Docking with Information on Evolutionary Conserved Interfaces.* Comput Struct Biol Workshop (CSBW) - IEEE BIBM Workshop, Atlanta, GA, November, 2011 (Abstract and Poster).

A23 Olson B^g and **Shehu, A***. *Local Minima Hopping Along the Protein Energy Surface.* IEEE Intl Conf on Biomed and Bioinf (BIBM), Atlanta, GA, November, 2011 (Abstract and Poster).

A22. Richardson SM, Olson B^g, Dymond JS, Burns R, Chandrasegaran S, Boeke JD, **Shehu A**, and Bader JS*. *Automated Design of Assemblable, Modular, Synthetic Chromosomes.* Annual RECOMB Satellite Meeting on Regulatory Genomics and Systems Biology, Boston, MA, 2009 (Abstract and Oral Presentation).

A21. Chung R^u, Jamil B^u, and **Shehu A***. *A Metropolis Monte Carlo Algorithm to compute Low-energy Structures of an RNA chain.* Grace Hopper Conference Celebration of Women in Computing, Tucson, Arizona, 2009 (Abstract and Poster).

A20. Mostaghim A^u, Veltri D^g, Majul A^g, and **Shehu A***. Aspiring Scientist Summer Internship Program (ASSIP) Poster Presentations, Manassas, Virginia, 2009 (Poster).

A19. Miles C^g and **Shehu A***. *Computing Symmetric HomoOligomeric Structures.* Intl Conf on Intelligent Systems for Molecular Biology & European Conf on Computational Biology (ISMB-EECB), Stockholm, Sweden, 2009 (Abstract and Poster).

A18-A1. These posters were the result of Shehu's research as a graduate and undergraduate student and can be found **here**.

OTHER PUBLICATIONS[7]

O14. Kabir A* and **Shehu A***. *GOProFormer: A Multi-modal Transformer Method for Gene Ontology Protein Function Prediction.* bioRxiv 10.1101/2022.10.20.513033, 2022.

O13. Kabir A* and **Shehu A***. *Transformer Neural Networks Attending to Both Sequence and Structure for Protein Prediction Tasks.* arXiv 2206.11057, 2022.

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[7]These are not peer-reviewed. In addition to select technical reports, this list includes internal pieces and ACM profiles I introduced in a new section of the ACM SIGBIO newsletter. The objective was to feature prominent researchers and raise awareness of timely research problems for the ACM SIGBIO community.

O12. Qiao W* and **Shehu A***. *Space Partitioning and Regression Mode Seeking via a Mean-Shift-Inspired Algorithm.* arXiv 2104.10103, 2021.

O11. Lu Y^g, Kamranfar P^g, and **Shehu A***. *Traffic Flow Forecasting with Maintenance Downtime via Multi-Channel Attention-Based Spatio-Temporal Graph Convolutional Networks.* arXiv 2110.01535, 2021.

O10. Guo X^g, Du Y^u, Tadepalli S^g, Zhao L, and **Shehu A***. *Generating Tertiary Protein Structures via an Interpretative Variational Autoencoder.* arXiv 2004.07119, 2021.

O9. Molloy K, Plaku E, and **Shehu A***. *ROMEO: A Plug-and-play Software Platform of Robotics-inspired Algorithms for Modeling Biomolecular Structures and Motions.* arXiv 1905.08331, 2019.

O8. **Shehu A***. *Investing in Our Undergraduate Students.* George Mason Review, April 26, 2019.

O7. **Shehu A***. *Will China surpass the US in AI technology? Mason experts weigh in.* The George, April 26, 2019.

O6. **Shehu A***. *Computer Scientist in Profile: Yang Zhang.* ACM SIGBIO Record 4(2), 2, 2014.

O5. **Shehu A***. *Computer Scientist in Profile: Bruce Donald.* ACM SIGBIO Record 4(1), 5-7, 2014.

O4. **Shehu A***. *Computational Biologist in Profile: Ruth Nussinov.* ACM SIGBIO Record 3(3), 12-14, 2013.

O3. **Shehu A***. *Computer Scientist in Profile: Mona Singh.* ACM SIGBIO Record 3(1), 26-27, 2013.

O2. Veltri D^g and **Shehu A***. *Elucidating Activity-related Physico-chemical Features in Antimicrobial Peptides.* Technical Report, GMU-CS-TR-2012-6, 2012.

O1. Miles C^g, Olson B^g, and **Shehu A***. *Geometry-based Computation of Symmetric Homo-oligomeric Protein Complexes.* Technical Report, GMU-CS-TR-2009-2, 2009.

INVITED TALKS

T93. *Enabling and Accelerating Scientific Discovery with Generative AI.* Invited Seminar, Lucy Family Institute for Data and Society, Notre Dame, April 03, 2024.

T92. *GenAI In Education.* Masterclass, Gen Next Education, KCG College of Technology, Chennai, January 25, 2024.

T91. *Of Small Molecules, Large Molecules, AI, and Generative AI.* Invited Seminar, Center for Genetic Medicine, Children's National Hospital, January 19, 2024.

T90. *Artificial Intelligence in the Age of Large Language Models.* Invited Talk, Vienna Area Branch of AAUW and the Patrick Henry Library of Vienna, January 06, 2024.

T89. *AI Redux: Opportunities and Dangers Ahead.* Invited Talk, Carlisle Towers, November 05, 2023.

T88. *AI & ML Beyond ChatGTP: From Education to Training and Careers in our AI-powered Digital Society.* Masterclass, Gen Next Education, October 20, 2023.

T87. *Artificial Intelligence after ChatGTP.* Invited Talk, George Mason Regional Library, Fairfax, VA, September 05, 2023.

T86. *How Can Artificial Intelligence (AI) Really Improve Our Lives?* Invited Talk, Prince William Chamber of Commerce Business Series, VA, May 09, 2023.

T85. *What Can Artificial Intelligence Tell Us About American Grand Strategy?* Session on Implications of Artificial Intelligence for Global Politics, International Studies Association (ISA) Annual Convention, Montreal, Canada, March 17, 2023 (with M Hunzeker).

T84. *The Institutional Determinants of National Artificial Intelligence Infrastructures, Session on Implications of Artificial Intelligence for Global Politics.* International Studies Association (ISA) Annual Convention, Montreal, Canada, March 17, 2023 (with JP Singh).

T83. *Are ChatBots ready for Business?* Dell Perspectives, February 01, 2023.

T82. *Representation Learning from Genotypes to Phenotypes: Linking Chemical and Biological Space in Small Molecules and Macromolecules.* Keynote, IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM), Las Vegas, NV, December 07, 2022.

T81. *AI for Human Biology and Health.* Radio Interview: A Structure Prediction Miracle, With Good Reason, WAMU 88.5FM, December 05, 2022.

T80. *Digital Innovation for Digital Therapeutics.* Keynote, International Symposium on Digital Therapeutics, George Mason University, Arlington, VA, November 09, 2022.

T79. *AI For Small and Large Molecules: From Foundational Insight to Understanding and Discoveries.* Keynote, 2022 Interdisciplinary Research Fall Forum, The Ohio State University, Columbus, OH, November 08, 2022.

T78. *Artificial Intelligence (AI): How did we Get Here, What is Here, and Where we are Heading.* Invited Talk, National Leadership Council, Middleburg, VA, October 29, 2022.

T77. *AI and our Digital Society.* Invited Talk, Science Tap Program, Loudon County Public Library, VA, October 06, 2022.

T76. *Digital Innovation For Good.* IDIA Presentation, George Mason University Board of Visitors Research Committee Report, Fairfax, VA, September 29, 2022.

T75. *The Cultural, Economic, and Institutional Determinants of AI Infrastructures and theirConsequences in Global Contexts.* PI Meeting Presentation, DoD Trust and Influence Program, VA, September 15, 2022.

T74. *Common Attributes of Responsive Proposals.* Invited Talk, 30th Conference for Intelligent Systems in Molecular Biology (ISMB), NIH-NSF Smart Health Program Special Track, Madison, WI, July 12, 2022.

T73. *Deep Learning for Molecular Biology.* Invited Short Talk, Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems Workshop, Tysons Corner, VA, June 23, 2022.

T72. *Small Molecule Generation with Property Control via Disentangled Representation Learning.* Key Speaker, AI for Bio & Medical Applications at TechConnect World Innovation Conference & Expo 2022 , June 14, 2022.

T71: *Negative Broader Impacts of Large Language Models.* Invited Talk, NVTC Impact AI Summit, Responsible AI by Design: The High Road of Mission AI at Scale Panel, Tysons Corner, VA, May 11, 2022.

T70. *The Journey to AlphaFold2.* AI Tea Series Talk, NSF, CISE, IIS, April 13, 2022.

T69. *AI/ML-Driven Scientific Advances: A Personal Journey, Lessons, and Outlook.* Invited Speaker, IEEE Technical Talk, IEEE Washington/Northern VA Computer Society Chapter, March 15, 2022.

T68. *Big Ideas and Big Data.* Invited Speaker, IEEE BigData, December 17, 2021.

T67. *How to Prepare a Successful Proposal for NSF CISE/IIS.* Invited Speaker, Early CAREER Workshop, Design Automation Conference (DAC), December 05, 2021.

T66. *Spatio-temporal machine learning in support of integrative biology.* Invited Speaker, AMIA Workshop on "Spatio-temporal informatics for Translational Bioinformatics", November 22, 2021.

T65. *Deep Learning for Linking Chemical and Biological Space in Small Molecules and Macromolecules.* AI Track Keynote, TechConnect World Innovation Conference & Expo 2021, October 19, 2021.

T64. *Computer Information, Science, and Engineering (CISE) Directorate.* Keynote, NSF Grant Conference, October 4-8, 2021.

T63. *From Genotypes to Phenotypes: Calling (Deep) Modelers to Step up their Game.* Keynote, 20th Internal Workshop on Data Mining in Bioinformatics (BIOKDD), held virtually in conjunction with SIGKDD 2021, August 15, 2021.

T62. *AI-Enabled Discovery of Macromolecular Structure, Dynamics, and Function.* Invited Talk, Chemical Theory Center Seminar Series, University of Minnesota, January 22, 2021.

T61. *Artificial Intelligence and Data.* Invited Talk, State Department's Great Decisions, Greenspring Retirement Community, Springfield, VA, December 15, 2020.

T60. *Great Disruptions and Expectations: A Perspective in Protein Modeling Research.* Keynote, 10th International Conference on Computational Advances in Bio and medical Sciences (ICCABS), December 12, 2020.

T59. *Physics- and Data-driven Studies of Macromolecules.* Invited Talk, Keck Center Celebration, Rice University, October 30, 2020.

T58. *A Data-driven Journey into Macromolecular Structure, Dynamics, and Function.* Invited Talk, NSF HDR Workshop on Knowledge Guided Machine Learning, August 20, 2020.

T57. *An AI-aided Entry to Modeling Actuated Systems.* AI Tea Series Seminar, NSF, CISE, IIS, April 22, 2020.

T46. *Discriminative and Generative Models of Protein Structure, Dynamics, and Function.* Invited Talk, Clarkson University, Potsdam, NY, April 19, 2019.

T45. *A Vision of Data-driven Discovery as the Bedrock of Convergence Research.* Invited Talk, NSF CISE/IIS, Alexandria, VA, February 06, 2019.

T44. *Recurrent Neural Networks, Generative Models, and Generative Adversarial Networks.* Invited Talk, Micron Corporation, Manassas, VA, August 24, 2018.

T43. *Nga Struktura, te Dinamika, dhe Funksioni i Sistemeve Molekulare dhe Inxhinerike me Algoritme Optimizimi dhe Analize Statistikore.* Invited Talk, Fakulteti i Shkencave, University of Tirana, June 29, 2018.

T42. *Biomolecules in Motion: Sample-based Models of Dynamics Elucidating Function and Mechanisms in the Healthy and Diseased Cell.* Invited Talk, Symposium on Data Science and Statistics, Reston, VA, May 18, 2018.

T41. *All about Energy Landscapes: Generating and Analyzing them to Predict and Characterize Protein Structure, Dynamics, and Function.* Invited Talk, Chemistry and Biochemistry Seminar, George Mason University, Fairfax, VA, April 16, 2018.

T40. *From Protein Structure to Dynamics and (Dys)Function via Energy Landscapes.* Invited Talk, IEEE Intl Conf on Bioinformatics and Biomedicine (BIBM), Kansas City, MO, November 15, 2017.

T39. *From Mutations to Mechanisms and Dysfunction via Computation and Mining of Protein Energy Landscapes.* Competitively-accepted Oral Presentation, 3DSIG Satellite Meeting, Intel Mol Sys Biol (ISMB), Prague, Czech Republic, July 21, 2017.

T38. *Data-driven Stochastic Optimization for Sample-based Models of Protein Energy Landscapes.* Contributed Talk, Workshop on Energy Landscapes: Structure, Dynamics and Exploration Algorithms[8], Telluride, CO, July 17-21, 2017.

T37. *Exploration Bias in Modeling Protein Equilibrium Dynamics.* Invited Talk, University of Zurich, Zurich, Switzerland, July 12, 2017.

T36. *Sample-based Models of (Altered) Protein Energy Landscapes Reveal much about (Dys)Function.* Invited Talk, Laboratory of Computational Biology Seminar Series, National Heart, Lung and Blood Institute, NIH, June 29, 2017.

T35. *Of Form and Function: Stochastic Optimization Elucidates Role of Dynamics in Proteinopathies.* Invited Talk, Krasnow Institute for Advanced Study, Seminar Series , George Mason University, February 20, 2017.

T34. *Sample-based Representations and Algorithms for Modeling Protein Structure and Dynamics.* Invited Talk, 6th Workshop on Logic and Systems Biology (LSB), 31st Annual ACM/IEEE Symposium on Logic in Computer Science (LICS), July 09, 2016.

T33. *Should Have Gone To Systems.* Invited Talk, Science Slam, Women@GECCO, Genet and Evol Comput Conf (GECCO), July 12, 2015.

T32. *Recovering Energy Landscapes and Mapping Functionally-relevant Structural Transitions.* Highlight Talk, Computational Structural Biology Workshop (CSBW), ACM Conf on Bioinf and Comput Biol (BCB), September 20, 2014.

T31. *Probabilistic Approaches to Unravel the Form to Function Relationship in Biomolecular Systems.* Seminar Series, Institute for Bioscience and Biotechnology Research (IBBR), Rockville, MD, March 10, 2014.

T30. *From the Nanoscale to the Petascale: Probabilistic Algorithmic Frameworks for Characterizing Complex Biomolecular Systems in the Presence of Constraints.* Biomedical Engineering Seminar Series, University of Florida, Gainesville, FL, January 9, 2014.

T29. *Advancing Biomolecular Modeling and Simulation: A Probabilistic Approach for Characterizing Complex Systems in the Presence of Constraints.* Volgenau School of Engineering Seminar, George Mason University, Fairfax, VA, October 17, 2013.

T28. *Probabilistic Approaches to Protein Modeling.* Mechanical Engineering Seminar Series, Johns Hopkins University, Baltimore, MD, February 14, 2013.

T27. *Genetic Programming Based Feature Generation for Automated Functional Analysis and Annotation of DNA Sequences.* Rocky Mountain Bioinformatics Conference, Aspen/Snowmass, Colorado, December 8, 2012, accepted oral presentation.

T26. *Probabilistic Search Frameworks for Protein Modeling.* School of Systems Biology Seminar, George Mason University, Fairfax, VA, November 20, 2012.

T25. *Of Protein Structures and Motions: Probabilistic Search and Optimization.* Applied and Computational Math Seminar, George Mason University, Fairfax, VA, November 2, 2012.

T24. *Probabilistic Search Frameworks for Modeling Structures and Motions of Protein Systems.* ACM BCB Invited Talk, Orlando, FL, October 8, 2012.

T23. *Stochastic Search to Map the Space of Local Minima in the Protein Energy Surface.* Fox Chase Cancer Center, Philadelphia, PA, October 2012.

T22. *Novel Perspectives on Exploring the Protein Conformational Space for Characterizing Structures and Motions in Protein Systems.* College of Information Science Seminar, Drexel University, Philadelphia, PA, October 2012.

T21. *Probabilistic Methods for Structural Characterization of Protein Systems.* Computer Science Seminar, Northern Virginia Center, Virginia Tech, Falls Church, VA, March 16, 2012.

T20. *Novel Algorithmic Frameworks for Protein Conformational Search.* Bioengineering Department Seminar, UMD, College Park, MD, February 10, 2012.

T19. *Simplifying and Sampling the Protein Conformational Space.* Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, February 6, 2012.

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[8]The workshop is a yearly event and is structured like Dagstuhl seminar series, quizzing speakers on results, ideas, sketches, and open problems anywhere from 45 minutes to 2 hours.

T18. *Probabilistic Frameworks for Protein Conformational Search: Characterization of Native Structures of Protein Chains and Protein-based Assemblies.* Rocky Mountain Bioinformatics Conf, Aspen/Snowmass, Colorado, December 10, 2011.

T17. *Probabilistic Search Frameworks for Modeling Structures, Motions, and Assembly of Protein Molecules.* Computational Materials Science Center Colloquium, George Mason University, Fairfax, VA, November 28, 2011.

T16. *Probabilistic Search Algorithms to Compute Conformations of the Protein Native State.* Chemistry Department Seminar, GMU, Fairfax, VA, September 29, 2011.

T15. *A Probabilistic Framework for the Characterization of the Protein Native State.* Computer Science Seminar, Lehigh University, Bethlehem, PA, March 16, 2011.

T14. *Combining Evolutionary Algorithms with Supervised Learning to Extract Signals from Biological Data.* BioLearn Workshop, BIONETICS, Boston, MA, December 02, 2010.

T13. *Mapping Conformational Spaces of Protein Molecules.* Computer Science Seminar, University of Massachusetts at Boston, Boston, MA, December 01, 2010.

T12. *Characterizing Biological Systems at the Molecular Level.* ACE Scholars Research Highlights Invited Talk, George Mason University, Fairfax, VA, October 13, 2010.

T11. *Probabilistic Methods to Compute Biologically-active Protein Conformations.* Computer Science Seminar, College of William and Mary Williamsburg, VA, June 1, 2010.

T10. *Computational Aspects of Sequence, Structure, and Function in Protein Molecules.* NCBI CBB Seminar, NIH, MD, Jun 18, 2009.

T9. *Motions and Assembly of Biological Molecules.* ACE Scholars Program Seminar, George Mason University, VA, Mar 17, 2009.

T8. *Geometric Algorithms for Biological Research: Everything is a Puzzle After All.* GRAND Seminar Series, George Mason University, VA, Oct 16, 2008.

T7. *From Atoms to Molecules to Machines: Computing Protein Motions to Elucidate Function.* Bioinformatics Colloquium, George Mason University, VA, Oct 7, 2008.

T6. *A Multiscale Framework for the Characterization of Protein Native States.* National Meeting of the American Chemical Society (ACS), New Orleans, LA, Apr 6, 2008.

T5. *Computing Structural Flexibility in the Protein Native State.* University of Chicago, Chicago, IL, Feb 6, 2008.

T4. *Characterizing Native Flexibility in Proteins.* Fox Chase Cancer Center, Philadelphia, PA, Jan 23, 2008.

T3-T1. These talks were during Shehu's research as a graduate student and can be found **here**.

OTHER RESEARCH PRODUCTS

A complete list of web servers, source code, and executables accompanying various publications are available at **OurTools** on our **Our Computational Biology Lab Webpage**. Code and pre-trained models can be found at **https://github.com/amarda-shehu**. Additional community dissemination and outreach materials (including research and education) are also available on our laboratory webpage.

Selected Source-code, Executables, and Web Servers:

15. GOProFormer: A Multi-Modal Transformer Method for Gene Ontology Protein Function Prediction. Anowarul Kabir and Amarda Shehu. This work has appeared in Biomolecules 12(11):1709, 2022. Code and pre-trained model are available at https://github.com/amarda-shehu/GoProFormer.

14. Generating Tertiary Protein Structures via Interpretable Graph Variational Autoencoders. Xiaojie Guo, Yuanqi Du, Sivani Tadepalli, Liang Zhao, and Amarda Shehu. This work has appeared in Bioinformatics Advances 2021. Code is available at https://github.com/amarda-shehu/CO-VAE.

13. Generative Adversarial Learning of Protein Tertiary Structures. Taseef Rahman, Yuanqi Du, Liang Zhao, and Amarda Shehu. This work has appeared in Molecules 2021. Data and selected trained models are publicly available through IEEE Dataport (ieee-dataport.org) under DOI 10.21227/m8sa-cz14, 2021

12. ROMEO, Object-Oriented, Plug-n-Play Robotics-Inspired Protein Modeling, 2017

11. AMPScreen: Antimicrobial Recognition and Genome-wide Screening, 2016

10. SIfTER: A Structure-guided Memetic, Cellular, and Multiscale Evolutionary Algorithm for Mapping Protein Conformation Spaces, 2015

9. EFC-FCBF: Framework for Feature Construction and Selection for Improved Recognition of Antimicrobial Peptides, 2014

8. HEA-PSP: A Hybrid Evolutionary Search Framework with Various Crossover Implementations for Ab-initio Protein Structre Prediction, 2014

7. EFFECT: Framework for Automated Construction and Extraction of Features for Classification of Biological Sequences, 2013

6. Binary Response Models for Recognition of Antimicrobial Peptides, 2013

5. Statistical Model Building for Antimicrobial Peptide Recognition, 2013

4. Novel features for Antimicrobial Peptide Recognition, 2013

3. Spatial EA Framework for Parallel Machine Learning, 2012

2. An Evolutionary Algorithm For Feature Generation from Sequence Data, 2012

1. An Evolutionary Algorithm For SVM Kernel Optimization, 2011

CURRICULUM DEVELOPMENT

Curriculum Development:

CS695 - Network Science: Principles and Applications is a special topics graduate course I proposed and first taught in Fall 2016 in collaboration with Prof. Fei Li. The objective of this course is to introduce students to network-based treatments of complex systems and provide students with a broad but rigorous overview of network science. The course emphasizes the fundamental underpinnings of network science to graph-theoretic concepts and graph algorithms and covers a rich set of state-of-the-art algorithmic, computational, and statistical methods for diverse applications in communications, biology, ecology, brain science, sociology, economics, epidemiology, synchronization, adaptive network formation, and more.

CS689 - Planning Motions of Robots and Molecules is a new graduate course I proposed as a technical elective (CS795 - Geometric Algorithms for Bioinformatics) and taught first in Fall 2009. The first offering introduced modeling and simulation of biological systems through analogies with robotic mechanisms and motion planning. After discussions with students and robotics faculty exposed the need for a graduate robot motion planning course, I redesigned the course to focus on robot motion planning and present special applications on biological molecules. The course has been approved as a regular course, CS689. I now teach CS689 every three semesters.

CS444 - Introduction to Computational Biology is a new undergraduate course I proposed as a technical elective (CS499 - Bioinformatics and Computational Biology I) and taught in Spring 2009-2011. The course was cross-listed as ECE401 and BINF401 to gage student interest in new inter-departmental bioinformatics and bioengineering programs. With these goals in mind, the course provided a broad view of classic computational problems in sequence, structure, and systems biology. The course was very well received and has been approved as a regular course, CS444. I now teach CS444 every three semester.

List of Courses Taught at Mason:[9]

CS485 Autonomous Robotics	Fall 2018, 2016, 2013
CS580 Introduction to Artificial Intelligence	Spring 2018, 2016
CS689 Planning Motions of Robots and Molecules	Spring 2018, 2016, 2014, 2012
CS583 Analysis of Algorithms I	Spring 2019, Fall 2017, 2014, Spring 2013, Fall 2010, 2008
CS483 Analysis of Algorithms I	Spring 2017, 2010
CS695 Network Science: Principles and Applications	Fall 2016
CS444 Introduction to Computational Biology	Fall 2012, Spring 2011
CS499 Bioinformatics and Computational Biology I (cross-listed as BINF401, ECE499)	Spring 2010, 2009
CS795 Geometric Algorithms for Bioinformatics	Fall 2009

DISSERTATIONS AND THESES DIRECTING

Ph.D. Dissertations:

13 Rahman T. *Generative AI for Protein Modeling: Sampling Protein Conformation Space,* George Mason University, June 2023. Committee: Shehu A (dissertation director and chair), Kosecka J, Liu M, and Jiang W. *Now Teaching Assistant Professor at University of Central Florida.*

12 Alam F. F. *Deep Latent Variable Models for Learning Representations of Protein Tertiary Structures,* George Mason University, April 2023. Committee: Shehu A (dissertation director and chair), Duric Z, Anastasopolous A, and Qiao W. *Now Teaching Assistant Professor at University of Maryland College Park.*

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[9]I have been on teaching leave from George Mason University since August 19, 2019, to serve as IPA at the National Science Foundation in the III program in the IIS division in the CISE directorate.

11 Kamranfar P. *Machine Learning Enabled Health Monitoring and Diagnosis of Engineering Systems,* George Mason University, April 2023. Committee: Shehu A (dissertation director and chair), Lattanzi D, Barbara D, and Yao S. *Now Teaching Assistant Professor at George Mason University.*

10. Kabir K. L. *Unsupervised Learning for Molecular Structure Discoveries,* George Mason University, June 2022. Committee: Shehu A (dissertation director and chair), Duric Z, Yao S, and Qiao W. *Now Teaching Assistant Professor at Stevens Institute of Technology.*

9. Zaman A. *Evolutionary Techniques for De Novo Protein Conformation Ensemble Generation,* George Mason University, July 2021. Committee: Shehu A (dissertation director and chair), De Jong KA, Brodsky A, and Qiao W. *Now Teaching Assistant Professor at George Mason University.*

8. Rajabi Z. *Machine Learning over Social Media: From Unsupervised User Behavioral Models to Emotion Recognition via Deep Learning,* George Mason University, April 2021. Committee: Shehu A (dissertation director and chair), Uzuner O, Anastasopoulos A, and Zhao L. *Now Applied Data Scientist at Adobe.*
   Daniel Barbará, Wanli Qiao, and Fei Li. *Now Teaching Assistant Professor at University of Buffalo.*

7. Gogovi G. *Polymers and Biomolecules in Solvent: A Molecular Dynamics Study,* George Mason University, November 2020. Committee: Kinser J (committee chair), Shehu A (dissertation director), Kavak H, and Papaconstantopoulos DA. *Now Assistant Professor at University of Houston.*

6. Akhter N. *Summarization, Visualization, and Mining of Molecular Landscapes,* George Mason University, March 2020. Committee: Shehu A (dissertation director and chair), Barbará D, Qiao W, and Li F. *Now Teaching Assistant Professor at University of Buffalo.*

5. Veltri D. *A Computational and Statistical Framework for Screening Antimicrobial Peptides,* George Mason University, July 2013. Committee: Shehu A (dissertation director), Solka J (committee chair), Vaisman I, and Matthews B. *Now a Computational Genomics Specialist at NIH-NIAID.*

4. Hashmi I. *Probabilistic Approaches to Protein-protein Docking,* George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Rangwala H, Barbara D, and Kabbani N. *Now a Teaching Assistant Professor in IST Department at GMU.*

3. Molloy K. *Probabilistic Algorithms for Modeling Protein Structure and Dynamic,* George Mason University, January 2015. Committee: Shehu A (dissertation director and chair), Barbara D, Blaisten-Barojas E, and Lien J-M. *Now a tenure-track Assistant Professor at James Madison University.*

2. Kamath U. *Evolutionary Machine Learning Approach for Big Data Sequence Mining,* George Mason University, December 2013. Committee: De Jong KA (dissertation director and chair), **Shehu A** (dissertation co-advisor), Domeniconi C, and Arciszewski A. *Now Chief Analytics Officer at Digital Reasoning.*

1. Olson B. *Evolving Local Minima in the Protein Energy Surface,* George Mason University, July 2013. Committee: Shehu A (dissertation director and chair), De Jong KA, Blaisten-Barojas E, Kosecka J, and Lien J-M. *Now Engineering Manager, Machine Learning at LinkedIn.*

M.S. Theses:

8. Lu Y. *Predicting Traffic Speed Under the Impact of Maintenance Downtime with Graph Convolutional Networks,* George Mason University, February 2021. Committee: Shehu A (committee chair), Lattanzi D (thesis director), and Zoran Duric.

7. Sambare S. *Structure- and Energy-based Analysis of FGFR2 Kinase Mutations Revealing Differences in Cancer and Syndrome Mutations,* George Mason University, May 2019. Committee: Shehu A (thesis director), Seto D (committee chair), and Klimov D.

6. Morris D. *Snapshots and Springs: Analyzing and Reproducing the Motions of Molecules,* George Mason University, August 2017. Committee: Shehu A (thesis director and chair), Duric Z, and Molloy K.

5. Majul A. *Comparative Molecular Dynamic Simulations of 2 Helical AMPs Found in Snakes ATRA-1 and ATRA-2,* George Mason University, July 2015. Committee: Bishop B (committee chair), Shehu A (thesis director), and Mikell P.

4. Veltri D. *Sequence-based Classification of Antimicrobial Peptides,* George Mason University, March 2013. Committee: Shehu A (thesis director), Vaisman I (committee chair), and Bishop B.

3. Hashmi I. *A Probabilistic Search Algorithm for Protein-Protein Docking,* George Mason University, November 2012. Committee: Shehu A (thesis director and chair), De Jong K, and Lien J-M.

2. Olson B. *Probabilistic Search Algorithms for Protein Structure Prediction,* George Mason University, November 2011. Committee: Shehu A (thesis director and chair), Kosecka J, and Lien J-M.

1. Molloy K. *Variable-Length Fragment Assembly in a Probabilistic Protein Structure Prediction Framework,* George Mason University, June 2011. Committee: Shehu A (thesis director and chair), Duric Z, and Lien J-M.

DISSERTATION ADVISING

† Fardina Alam, (GMU, PhD Dissertation Pre-defense and Defense, committee chair: Amarda Shehu)   Spring 2023

† Parastoo Kamranfar, (GMU, PhD Dissertation Pre-defense and Defense, committee chair: Amarda Shehu)   Spring 2023

† Taseef Rahman, (GMU, PhD Dissertation Pre-defense and Defense, committee chair: Amarda Shehu)   Spring 2023

† Bahman Pedrood, (GMU, PhD Dissertation Pre-defense and Defense, committee chair: Carlotta Domeniconi)   Spring 2023

† Kourosh Teimouri Baghaei (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous)   Spring 2023

† Huayu Zhou (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous)   Spring 2023

† Samuel Blouir (GMU, Comprehensive Exam committee, chair: Antonios Anastasopolous)   Spring 2023

† Eric Scott, Computer Science, PhD Pre-defense, Committee Member (Committee Chair: Carlotta Domeniconi)   Summer 2022

† Abhisekh Rana, Computer Science, Comprehensive Exam (Committee Chair: Zoran Duric)   Spring 2022

† Taseef Rahman, PhD Proposal Defense Committee Chair   Spring 2022

† Toki Inan, Comprehensive Exam Committee Member   Spring 2022

† Jonathan Mbuya, Computer Science, Comprehensive Exam, Committee Chair,   Spring 2022

† Abhisekh Rana, Computer Science, Comprehensive Exam, Committee Member (Committee Chair: Carlotta Domeniconi),   Spring 2022

† Fardina Alam, Computer Science, PhD Proposal Committee Chair,   Spring 2021

† Lutful Kazi Kabir, Computer Science, PhD Pre-defense, Committee Chair   Fall 2021

† Tasfia Mashiat, Computer Science, Comprehensive Exam Committee Chair,   Fall 2021

† Bahman Pedrood, Computer Science, Comprehensive Exam and PhD Proposal Defense Committee Member (PhD Dissertation Director: Carlotta Domeniconi)   Spring – Summer 2021

† Jooyeon Lee, Information Sciences and Technology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2021-present

† Fatemah Husain, Information Sciences and Technology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2020-2021

† Sivani Tadepali, Computer Science, Comprehensive Exam Committee Member (Committee Chair: Huzefa Rangwala)   Spring 2021

† Lutful Kazi Kabir, Computer Science, Comprehensive Exam Committee Member (Committee Chair: Huzefa Rangwala)   Spring 2021

† Fardina Alam, Comprehensive Exam Committee Member (Committee Chair: Zoran Duric)   Spring 2021

† Anowarul Kabir, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Spring 2021

† Taseef Rahman, Comprehensive Exam Committee Member (Committee Chair: Jana Kosecka)   Spring 2021

† Zahra Rajabi, PhD Pre-Defense and Defense Committee Chair (PhD Dissertation Co-Director: Ozlem Uzuner)   Spring 2021

† Parastoo Kamranfar, PhD Proposal Defense Committee Chair (PhD Dissertation Director: David Lattanzi)   Spring 2021

† Zahra Rajabi, PhD Proposal Defense Committee Chair, (PhD Dissertation Co-Director: Ozlem Uzuner)   Fall 2020

† John Hamre, School of Systems Biology, PhD Pre-defense and Defense Committee Member (PhD Dissertation Director: Saleet Jafri)   2020-2021

† Xiaojie Guo, Information Sciences and Technology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Liang Zhao)   2019-2021

† Angela Achary, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

† Yong Yang, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

† Manpriya Dua, Comprehensive Exam Committee Member (Committee Chair: Huzefa Rangwala)   Fall 2020

† Li Zhang, Comprehensive Exam Committee Member (Committee Chair: Carlotta Domeniconi)   Fall 2020

† Parastoo Kamranfar, Comprehensive Exam Committee Member (Committee Chair: Jessica Lin),   Fall 2020

† Xavier Gitiaux, Comprehensive Exam Committee Member (Committee Chair: Jana Kosecka)   Spring 2020

† Zahra Rajabi, Comprehensive Exam Committee Chair   Spring 2020

† Ahmed ElMolla, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Sean Luke)   2019

† Kahyun Lee, Information Sciences and Technology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Ozlem Uzuner)   2019-2021

† Gideon Gogovi, CMASC, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Estela Blaisten-Barojas)   2018-2021

† Jing Lei, Statistics, PhD Proposal Committee Member (PhD Dissertation Director: Wanli Qiao)   2018-2020

† Joseph Graus, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Yotam Gingold)   2018-2019

† Achyuthan J.R., Civil, Environmental, and Infrastructure Engineering, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: David Lattanzi)   2018-2016

† Christopher Siwy, School of Systems Biology, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Dmitri Klimov)   2017-2014

† Gregory Helmick, CSI, PhD Proposal Committee Member (PhD Dissertation Director: Estela Blaisten-Barojas)   2017-2014

† Evan Behar, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien)   2017-2013

† Zhonghua Xi, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien)   2017-2015

† Yoseph Abere, CSI, PhD Proposal and Pre-defense Committee Member (PhD Dissertation Director: Estela Blaisten-Barojas)   2017-2015

† Jose Colbes, Computer Science, CICESE-Mexico, PhD Proposal Committee Member (PhD Dissertation Director: Carlos Brizuela)   2015-2014

† Yanyan Lu, Computer Science, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Jyh-Ming Lien)   2013-2012

† Adam Cadien, SPACS, PhD Proposal, Pre-defense, and Defense Committee Member (PhD Dissertation Director: Howard Sheng)   2015-2012

† Nada Basit, Computer Science, PhD Proposal Committee Member (PhD Dissertation Director: Harry Wechsler)   2011

STUDENT ADVISING AND MENTORING   (in research-related activities)

Postdoctoral Fellows:

3. Pourya Hoseini (Fall 2020)
2. Tatiana Maximova (May 2018 - April 2015)
1. Emmanuel Sapin (December 2016 - January 2015)

Ph.D. Students:[10]

23. Samuel Blouir (Spring 2023–present)
24. Asher Moldwin (Spring 2023–present)
22. Dhiman Goswami (Fall 2021–Spring 2023)
21. Yuanjie Lu (Fall 2021–Spring 2023)
20. Shiva Ghaemi (Fall 2021–present)
19. Anowarul Kabir (Fall 2020–present)
18. Toki Inan (Spring 2020–present)
17. Megan Herceg (Summer 2019–present

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[10]These students have earned numerous awards during their research in my lab, some of which are highlighted below.

16. Taseef Rahman (Spring 2019–present)

15. Fardina Alam (Spring 2019–present)

14. Yiyang (Alex) Lian (Fall 2018–2021)

13. Parastoo Kamranfar (Summer 2018–present)

12. Manpriya Dua (Summer 2018–present)

11.-1. Ph.D. alumni: Kazi Lutful Kabir, Ahmed Bin Zaman, Gideon Gogovi, Zahra Rajabi, Nasrin Akhter, Erich O'Saben, Daniel Veltri, Irina Hashmi, Kevin Molloy, Uday Kamath, and Brian Olson.

M.S. Students:

14. Sree Ram GabbiReddy, CS	2024–present
13. Yuanjie Lu, CS	2019–2021
12. Sivani Tadepalli, CS	2018–2021
11. Sabiha Salma, CS	2020–2021
10. Prasanna Venkatesh Parthasarathy, CS	2019-2018
9. Suma Dixit, CS	2019-2018
8. Snehal Sambare, CS	2019-2018
7. Liban Hassan, CS	2018-2017
6. David Morris, CS	2017-2016
5. Ryan Moffatt, CS	2016-2015
4. Rudy Clausen, CS, now at Parsons	2015-2012
3. Amr Majul, School of Systems Biology, now at MITRE	2013
2. Seyed Farid Hendi, CS, now at Appian	2011
1. Christopher Miles, CS, now at Google	2010

Undergraduate Students:[11]

38. Alejandro Capecchi Perez (Statistics)	Fall 2021 - present
37. Sanela Refai (BIO)	Fall 2021 - present
36. **Yinkai Wang** (CS)	Fall 2021 - present
35. Aowei Ding (CS)	Fall 2021 - present
34. Melanie Gipson, REU student from Georgia State University,	Summer 2021
33. Alex Felleson, REU student from Kenyon College,	Summer 2021
32. **Yuanqi Du** (CS)	Spring 2020 - present
31. Laura Alvarez (CS, Carlos III University of Madrid)	Spring 2019 - present
30. Carlos Guerra (CS)	Spring 2019 - present
29. Mansour Faragal (CS)	Spring 2019 - present
28. Cody Barrett (CS)	Spring 2019 - Summer 2018
27. Bakr Marou (CS)	Summer 2018
26. Michael Largent (CS, Indiana Institute of Technology)	Summer 2018
25. Connor Reguero (CS)	Fall 2017
24. Armen Hagopian (CS)	Summer 2017
23. Lu Lu, GMU (CS)	Summer 2017
22. **Xiaowen Fang**, GMU (CS)	Summer 2017
21. Erica Molinar, GMU (CS)	Spring 2017 - Fall 2016
20. Savindi Ranasinghe, GMU (CS)	Spring 2017 - Fall 2016
19. Bradley English, GMU (CSS/Neuroscience)	Spring 2017 - Fall 2016
18. Heather Hendy, GMU (CS)	Summer 2015 - Fall 2015
17. Jeffrey Horowitz, Rice University (CS)	Summer 2015
16. Mazyar Katouzian, GMU (CS)	Spring 2015 - Fall 2014

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[11]Mentoring of college and pre-college students and their inclusion in my lab's research activities is an important component of my scholarship at Mason. These students have co-authored refereed articles (students with names in bold), some even in first-author capacity, and have earned numerous awards, some of which are listed below.

15. Songyue Huang, GMU (CS)	Spring 2015 - Fall 2014
14. Wint Hnin, CRA-W DREU student from Cornell College (CS)	Summer 2014
13. Herath Pilapitiya, GMU (CS)	Summer 2014 - Spring 2014
12. Ruxi Xiang, GMU (CS)	Spring 2015 - Fall 2013
11. Mahmoud Namazi, GMU (Math)	Spring 2015 - Fall 2013
10. **Jennifer Van**, GMU (CS)	Summer 2014 - Fall 2012
9. **Sameh Saleh**, GMU (ACS Bioinformatics)	Spring 2013 - Fall 2011
8. Bryn Reinstadler , CRAW-DREU student from Williams College (CS)	Summer 2012
7. Subeer Talapatra, UVA (Chemical Engineering)	Summer 2012
6. Talhah Zafar, GMU (CS)	Summer 2012
5. Justin Towson, GMU (Neuroscience)	Spring 2011 - Fall 2010
4. **Jack Compton**, GMU (CS)	Spring 2011 - Fall 2010
3. Beenish Jamil, GMU (ACS Bioinformatics)	Summer 2010 - Spring 2009
2. Rachael Chung, CRA-W DREU student from UNCC	Summer 2009
1. Anahita Mostaghim, ASSIP fellow from UVA.	Summer 2009

High-School Students:[12]

19. Sofia Jacik, Riverside High School	Spring 2023
18. Shaurya Singh, Riverside High School	Spring 2023
17. **Vedant Vajre**, Stone Bridge High School	Summer 2021
16. Hailena Bian, Thomas Jefferson High School	Summer-Fall 2021
15. Spencer Huang, BASIS Independent McLean	Spring-Fall 2021
14. Alan Zhang, Thomas Jefferson High School	Fall 2020 - Spring 2021
13. Demian Yutin, Thomas Jefferson High School	Spring 2019 - Fall 2018
12. Fiona Carcani, Thomas Jefferson High School	Spring 2018 - Summer 2017
11. Noah Prinzbach, West Potomac High School	Summer 2017
10. **Sharmila Roy**, Thomas Jefferson High School	Summer 2018 - Summer 2017
9. Kevin Zou, Thomas Jefferson High School	Spring 2018 - Summer 2017
8. Rishin Pandit, Thomas Jefferson High School	Summer 2017
7. Neha Damaraju, Thomas Jefferson High School	Summer 2017
6. **Rohan Pandit**, Thomas Jefferson High School	Spring 2016 - Summer 2014
5. Pranay Singh, Thomas Jefferson High School	Summer 2014, 2012
4. Scott Jordan, ASSIP fellow, W. T. Woodson High School	Summer 2012
3. Niraja Bohidar, Thomas Jefferson High School	Summer-Fall 2012
2. Nakkul Sreenivas, Chantilly High School	2012-2011
1. Subeer Talapatra, Thomas Jefferson High School	Summer 2010

Selected Student Awards (grouped by student):

26. Fardina Fathmiul Alam (Ph.D. student), Outstanding PhD Dissertation Award, Computer Science	2023
25. Ahmed Bin Zaman (Ph.D. student), Computer Science Distinguished Academic Achievement Award	2021
24. Nasrin Akhter (Ph.D. student) Department of Computer Science Outstanding Graduate Student Award	May 2019
23. Kazi Lutful Kabir (Ph.D. student) Best Paper Award, BICOB	May 2019
22. Sharmila Roychoudhoury (TJ high-school student) Honorable Mention Poster at ACM BCB	August 2018
21. Tatiana Maximova (CS postdoctoral fellow) Outstanding research presentation at ISMB 3DSIG	July 2016
20. Bradley English (CSS/Neuroscience undergrad) OSCAR undergraduate apprenticeship	Fall 2016

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[12]I am a Thomas Jefferson Summer/Fall Program Mentor since 2014.

19. Heather Hendy (CS undergrad)
    OSCAR undergraduate apprenticeship   Spring 2016

18. Mazyar Katouzian (CS undergrad, graduated May 2015)
    OSCAR undergraduate apprenticeship   Spring 2015

17. Songyue Huang (CS undergrad, graduates May 2016)
    OSCAR undergraduate apprenticeship   Spring 2015

16. Daniel Veltri (School of Systems Biology Ph.D., graduated 2015)
    Best student paper at IEEE BIBM in first-author capacity   November 2014
    Travel Award, ICCABS   June 2013
    Outstanding Oral Presentation, School of Systems Biology Student Research Day, Daniel Veltri   May 2013

15. Irina Hashmi (CS Ph.D., graduated 2015)
    Best Poster Award, IEEE BIBM   October 2012
    Travel Awards, IEEE BIBM, CRA-W Grad Cohort Workshop   May 2011
    Research Assistant Fellowship   2010 - 2011

14. Rudy Clausen (M.S. Ph.D., graduated 2015)
    Guest (Intern) Researcher in the Cancer and Inflammation Program at the National Cancer Institute 2013-2014

13. Jennifer M. Van (CS undegrad, graduated 2015)
    Dean's Award in Physical Sciences at the College of Science Undergraduate Research Symposium   2014
    Oustanding Project Award at the Volgenau School of Engineering Undergraduate Research Celebration   2014
    Second author of a journal paper   2014
    Second author of a refereed conference paper   2013
    Princeton MOL/QCB Summer Program   May 2013
    CRA-W DREU (Distributed Research Experiences for Undergraduates)   May 2013
    University of Wisconsin Madison REU   May 2013
    OSCAR undergraduate apprenticeship   Spring 2013

12. Kevin Molloy (CS Ph.D., graduated 2015)
    Outstanding CS Graduate Student Award   April 2015
    Finalist for best paper award at BiCoB   March 2014
    Travel Award, ICCABS   June 2013
    Outstanding Academic Achievement Award   August 2011
    Dean Fellowship   Fall 2011 - Spring 2012
    Best Paper award at BIONETICS in second-author capacity   December 2010

11. Uday Kamath (IT Ph.D., co-advised with K. De Jong, graduated 2014)
    Honorable Mention, Humies Competition Award at GECCO   June 2012

10. Herath Pilapitiya (CS undegrad, graduated 2014)
    OSCAR undergraduate apprenticeship   Summer Intensive 2014

9. Brian Olson (CS Ph.D., graduated 2013)
    Mason VSE Outstanding Graduate Student Award   April 2013
    Outstanding Academic Achievement Award   May 2012
    Best Paper Award at BIONETICS in first-author capacity   December, 2010

8. Sameh Saleh (CS undergrad, graduated May 2013)
    First author of a refereed journal and a refereed workshop paper   2013-2012
    Second author of a refereed journal paper   2013
    Author of numerous abstracts and extended abstracts   2013-2012
    Finalist, Male, CRA Outstanding Undergraduate Researcher Award   May 2013
    Mason OSCAR Outstanding Undergraduate Research Award   May 2013
    Selected undergraduate presenter, NCUR   May 2013
    Keynote undergraduate speaker at COS Undergraduate Research Colloquium   May 2012
    OSCAR undergraduate apprenticeship   Fall 2011

7. Bryn Reinstadler (CS Williams College, graduated 2014)
    CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab   May 2012

6. Scott Jordan (Woodson high school, now at RIT)
    ASSIP high-school fellowship   June 2012

5. Justin Towson (CS undergraduate, graduated 2012)
    OSCAR undergraduate apprenticeship   Fall 2010

4. Jack Compton (CS Ph.D., graduated 2011)
    Second author of a refereed journal paper   2012

3. Beenish Jamil (CS undergraduate, graduated 2011)
   Honorable Mention, CRA Outstanding Undergraduate Research Award   May 2011
   CRA-W DREU (Distributed Research Experiences for Undergraduates)   May 2011

2. Rachael Chung (CS undergradute, UNCC, now CS Ph.D.)
   CRA-W DREU (Distributed Research Experiences for Undergraduates) in Shehu Lab   May 2009

1. Anahita Mostaghim
   ASSIP undergraduate fellowship   June 2009

DEPARTMENTAL AND UNIVERSITY SERVICE

University Service:

† Member of the Office of Research Innovation and Economic Impact (ORIEI) Research Leadership and Research Council, 2022-present.

† Member of Fuse TTIP Infrastructure Committee, 2023-present

† Member of Provost Search Committee, 2023.

† Member of TTIP Public Policy, AI, and Social Justice Faculty Search Committee, 2023.

† Member of Research Advancement Committee, 2022-present

† Member of University Institutes Strategic Planning Committee, 2022-present

† Member of University Communications Planning Committee, 2022-present

† Member of Fuse-Mason Square Programmatic Planning Committee, 2022-present

† Member of ORIEI Strategic Planning and Initiatives Search Committee, 2022.

† Member of ORIEI Executive Assistant Search Committee, 2022.

† Member of TTIP Ethics and AI Faculty Search Committee, 2022.

† Mentor of SCHEV Candidates, 2022.

† Member of Presidential Awards Review Committee 2021-2022.

† Member of TTIP AI & Society Search Committee, 2021-2022.

† Member of TTIP Computational Biomedicine Search Committee, 2021-2022.

† Conceptualizer and CS lead of cross-Mason working group of "Ethics and AI" – Proposed Transdisciplinary Undergraduate Minor, winner of Curriculum Impact Grant in Spring 2021 (together with Jesse Kirkpatrick, Alexander Monea, Rachel Jones, and Peng Warweg).

† Member of Tech Talent Investment Program (TTIP) Thematic Hiring Winning Team for AI & Society, 2020.

† Member of Advanced Computational Research Infrastructure Steering Committee, GMU, 2020.

† Member of Working Group, Envisioning Retreat, GMU School of Medicine, August 2019.

† Member of School of Computing Planning Committee, 2019.

† Member of University Research Advisory Committee, 2018-2019.

† Portfolio Consultant, Teaching Excellence Awards, 2018-2019.

† Steering/Advisory Board member for Office of Research Computing, 2017-2018.

† Organizer of cross-university Network Science Group (with Prof. Fei Li), January 2017-2018.

† GMU-INOVA Bioinformatics and Genomics Working Meeting (presenter), May 15, 2017.

† Mentor for Mason NSF CAREER program, March-July 2017.

† GMU NSF Career Workshop (panel member), 2019, 2018, 2017, 2012.

† University Scholars Selection Committee, February 20, 2016.

† Cyber and Computer Mason Multidisciplinary Grants Review Panel, July 16, 2015.

† Student Scholarly Activities subcommittee of the Mason Students as Scholars QEP Leadership Council, 2016-2013.

† GMU Research Highlight Series (presenter), ACE Scholars 2011, 2009.

College of Engineering and Computing Service:

† Member of CEC Research Council, 2020-present.

† Member of GMU CEC Computational Systems Biomedicine Search Committee, 2021-2022.

† Recruitment Committee Member, Department of Information Sciences and Technology, 2021-2022.

† Chair Recruitment Committee, Department of Computer Science, 2019.

† Chair Recruitment Committee, Department of Statistics, 2019.

† Recruitment Committee, Department of Statistics, 2017, 2016.

† Bioengineering SCHEV application, undergraduate curriculum in newly formed department, and program design prior to being a department, 2012-2008.

† Faculty recruitment subcommittee, Department of Bioengineering, 2008-2012.

Computer Science Department Service:

† Ideator and Co-organizer of "Ask Me Anything" series targeting Assistant Professors, GMU Computer Science Department 2020-2023.

† Ideator and Co-organizer of AI Tea Series Seminar, GMU Computer Science Department 2020-2023.

† AI Lab Coordinator, Department of Computer Science, 2020-present.

† Executive Committee Member, Department of Computer Science, 2020-present.

† Recruitment Committee, Department of Computer Science, 2019, 2018, 2017.

† Co-chair of GMU CS Distinguished Lecture Series organization committee 2018–2019.

† Member of GMU CS Advisory Council, 2018-2019.

† Member of GMU CS faculty evaluation committee, 2018-2019.

† Mentor of junior faculty, 2019, 2018, 2017.

† Co-organizer of Ph.D. research symposium (with Hakan Aydin, Huzefa Rangwala, and Yotam Gingold) 2015-2019.

† Co-designer of Foundations of CS qualification exam for advancement to Ph.D. candidacy, 2016-2019.

† Co-organizer of CS Ph.D. research symposium (with Jana Kosecka), 2015-2016.

† Co-organizer (with Jana Kosecka) of CS Seminar, George Mason University, 2014-2018

† Graduate Studies Committee, 2016-2019

† Ph.D. Committee, 2014-2019

† Faculty Evaluation Committee, 2017-2019

† Executive Committee, George Mason University, 2016-2014.

† Strategic Vision and Planning Committee, George Mason University, 2014.

† Ph.D. & IT Qualifying Exam (Foundations) Preparation Committee, 2013-2019.

† Ph.D. Admissions Committee, George Mason University, 2012-2019.

† Undergraduate Studies Committee, 2009-2011.

† Subcommittee to revise the Applied Computer Science degree in Biology into the new ACS degree in Bioinformatics, 2008-2011.

Contributions as Invitee and Host to School and Departmental Seminars:

† Aidong Zhang, University of Virginia	Distinguished Lecture Series, Fall 2022
† Mona Singh, Princeton University	Distinguished Lecture Series, Spring 2019
† Pierre Baldi, University of California at Irvine	Distinguished Lecture Series, Spring 2019
† Hadas Kress-Gazit, Cornell University	Distinguished Lecture Series, Fall 2017
† Jeremy Goecks, George Washington University	GRAND Seminar, Fall 2014
† Amina Woods, NIH	Bioengineering Seminar, Fall 2013
† Lydia Kavraki, Rice University	CS Distinguished Lecture Series, Spring 2013
† Philip Bryant, UMD College Park	Bioengineering Seminar, Spring 2013
† Silvina Matysiak, UMD College Park	Bioengineering Seminar, Spring 2012
† Claire Monteleoni, George Washington University	CS GRAND Seminar, Spring 2012
† Brian Chen, Lehigh University	CS GRAND Seminar, Fall 2011
† Anna Panchenko, NIH	CS GRAND Seminar, Fall 2009
† Rezarta Islamaj-Dogan, NIH	CS GRAND Seminar, Fall 2009

PROFESSIONAL SERVICE

Media Activities:

† Mason professors are researching hacker psychology to defend against cyberattacks. The George, May 02, 2024.

† Generative AI and Transformed Economies. Fairfax County Times, February 2024.

† How generative AI tools like ChatGPT could revolutionize business. Dell Perspectives, March 01, 2023.

† AI for Human Biology and Health: A Structure Prediction Miracle. With Good Reason, WAMU 88.5FM, December 05, 2022.

† International Symposium on Digital Therapeutics. DNews, November 11, 2022.

† Korea-US Digital Therapy Policy Symposium. Knews1, November 10, 2022.

Taskforces:

† Taskforce on 'Generative AI Risks and Associated Controls' in NIST AISIC Risk Management Working Group, member, 2024.

† Taskforce on 'Case Studies, Best practices, Piloting, and Reference Implementations of a GAI profile of the NIST AI RMF (NIST AI 100-1)' in NIST AISIC Risk Management Working Group, member, 2024.

† State Council of Higher Education for Virginia EO30 Taskforce.

Editorial Positions:

† Guest Editor of International Journal of Molecular Sciences (IJMS, IF: 6.208) Special Issue on Deep Learning for Modeling the Structure, Dynamics, and Function of Small and Large Molecules, 2022-2023.

† Guest Lead Editor of International Journal of Molecular Sciences (IJMS, IF: 6.208) Special Issue on Recent Advances in Computational Structural Bioinformatics, 2022-2023.

† Co-editor of Section on Theory and Simulation/Computational Methods in the Current Opinion in Structural Biology Journal, 2019-2021.

† Associate Editor of IEEE/ACM Trans Comput Biol & Bioinf Journal, April 2017-present.

† Guest Editor of Biomolecules, 2019-2018, special issue.

† Guest Co-editor of IEEE/ACM Trans Comput Biol & Bioinf Journal, 2017-2018 (special issue of ACM-BCB 2017)

† Guest co-editor, J Biomedical and Health Informatics 2017-2018 (special issue of ACM-BCB 2017).

† Guest Editor of PLoS Comput Biol, May 2017.

† Editorial board member, Intl J. of Data Mining and Bioinformatics (IJDMb), 2012-2017.

† Guest Co-editor of special collection on Macromolecular Structure and Dynamics of PLoS Comput Biol 2015.

† Co-editor of Robotica 2015 (special issue).

† Co-editor of IEEE/ACM Trans Comput Biol and Bioinf 2015 (special issue).

† Co-editor of J Comput Biol 2015 (special issue).

† Guest associate editor of Education Collection of PLoS Comput Biol 2014.

† Co-editor of BMC Struct Biol 2013 (special issue).

† Co-editor of J Bioinf and Comp Biol 2012 (special issue).

† Co-editor of J Bioinf and Comp Biol 2011 (special issue).

Organization of Workshops and Tutorials:

† "LLMs4Bio" Workshop at AAAI 2024, Vancouver, Canada.

† "Ethics and AI Undergraduate Minor at George Mason University: Planning Workshop" at George Mason University, March 25, 2022. (with Jesse Kirkpatrick/Philosophy, Alexander Monea/English, Rachel Jones/Philosophy, and Peng Warweg/CAHMP).

† "Spatial & Spatial-Temporal informatics: Methods, Tools and Emerging Opportunities for Translational Bioinformatics" Workshop (W23) at AMIA 2021 Annual Symposium, October 31, 2021, San Diego, CA. (with Arvind Rao/U Michigan Ann Arbor, Mary Saltz/Stony Brook, Shashi Shekhar/U Minnesota, Joel Saltz/Stony Brook Medicine, and Li Zhu/NIH).

† "Modeling Macromolecular Structures and Motions: Computational Methods for Sampling and Analysis of Energy Landscapes" Tutorial at ACM BCB 2018, Washington, DC.

† "Computational Structural Biology Workshop" at ACM BCB, August 20, 2017, Boston, MA.

† "Women@GECCO" Workshop at GECCO, July 15, 2017, Berlin, Germany.

† "Evolutionary Computation in Computational Biology" Workshop at GECCO, July 16, 2017, Berlin, Germany.

† "Robotics-inspired Algorithms for Modeling Protein Structures and Motions" Tutorial at ACM BCB 2017, Boston, MA.

† "Women@GECCO" Workshop at GECCO, July 2016, Denver, Colorado.

† "Evolutionary Computation in Computational Biology" Workshop at GECCO, July 2016, Denver, Colorado.

† "Evolutionary Algorithms for Protein Structure Modeling" Tutorial at ACM BCB, October 2016, Seattle, Washington.

† 10. "Computational Structural Biology Workshop" at IEEE BIBM, November 11, 2015, Washington, D.C.

† "Evolutionary Computation in Computational Biology" Workshop at GECCO, July 11, 2015, Madrid, Spain.

† "Evolutionary Algorithms for Protein Structure Modeling" Tutorial at GECCO, July 11, 2015, Madrid, Spain.

† "Computational Structural Biology Workshop" at ACM BCB, September 20, 2014, Newport Beach, LA.

† "Robot Motion Planning Methods for Modeling Structures and Motions of Biomolecules" Tutorial at ACM BCB, September 20, 2014, Newport Beach, CA.

† "Evolutionary Search Algorithms for Protein Modeling: From De-novo Structure Prediction to Comprehensive Maps of Functionally-relevant Structures of Protein Chains and Assemblies" Tutorial at GECCO, July 12, 2014, Vancouver, Canada.

† "NSF CISE CAREER Writing Workshop" March 31, 2013, Arlington, VA.

† "Artificial Intelligence and Robotics Methods in Computational Biology" Workshop at AAAI, July 14, 2013 Bellevue, WA.

† "Computational Structural Biology Workshop" at ACM BCB, September 22, 2013, Washington, D.C.

† "From Robot Motion Planning to Modeling Structures and Motions of Biological Molecules" Tutorial at ACM BCB, September 22, 2013, Washington, D.C.

† "Computational Structural Biology Workshop" at IEEE BIBM, October 4, 2012, Philadelphia, PA.

† "Computational Structural Biology Workshop" at IEEE BIBM, November 12, 2011, Atlanta, GA.

† "Evolutionary Computation and Machine Learning in Bioinformatics Workshop" (BioLearn) at BIONETICS, Dec. 1-3, 2010, Boston, MA.

Other Chairships:

† Chair of ACM/IEEE Trans Bioinf and Comp Biol (TCBB) Steering Committee, ACM representative, 2018-2022

† Session Chair of AI for Biomedical Applications Track, Tech Connect World Innovation and Expo 2021, National Harbor, MD.

† Senior Program Committee Member of KDD 2020, San Diego, CA.

† Tutorial chair of ISMCO 2019, Lake Tahoe, NV.

† General chair of ACM BCB 2018, Washington, D.C.

† Program co-chair of ACM BCB 2017, Boston, MA.

† "Undergraduate research highlights" section writer of ACM SIBIO newsletter, 2017.

† Program co-chair of IEEE BIBM 2015, Washington, D. C.

† Tutorials co-chair of ACM BCB 2014, Newport Beach, CA.

† "Computer Scientist in Profile" section writer of ACM SIGBIO newsletter, 2012-2014.

† Local arrangement chair of ACM BCB, Washington, D.C, September 22-25, 2013.

† Chair of Systems Biology session, ACM BCB, October 9, 2012.

† Co-chair of Poster Session at IEEE BIBM, October 4-7, 2012.

† Organizing Committee vice-chair of BIONETICS, Dec. 1-3, 2010.

† Co-organizer of Bioinformatics track of BIONETICS, Dec. 1-3, 2010.

Referee Activities[13]

† Grant proposal referee for Netherlands Organization for Scientific Research; Multidisciplinary University Research Initiative, Army Research Office; Spark Initiative, Swiss National Science Foundation; Advanced Research Projects Agency - Energy (ARPA-E); National Defense Science and Engineering Graduate Fellowships; NSF panels CISE-IIS, CISE-FET, CISE-CCF, CISE-CSSI, CISE-SI2, BIO-MCB; NIH study sections NINDS NST-2 (K99/R00 and F32); ZRG1 Special Emphasis S10 (study section chair); BST-80 AREA (R15) Bioengineering; BDMA, Special Emphasis Panel (SEP) for Biomedical Research Shared Instrumentation (S10); Bioinformatics - Topics in Computational Biosciences Special Emphasis Shared and High-End Instrumentation; Accelerating Scientific Discovery (ASDI) (Netherlands e-Science Center + Netherlands Organisation for Scientific Research); AgreenSkills (EU + INRIA).

† Journal paper referee for Nature Methods, Nature Communications, FEBS Letters, Bioinformatics, PLoS Comput Biol, PLoS One, J Phys Chem Lett, Scientific Reports, F1000 Research, BMC Genomics, Proteins: Struct, Funct, and Bioinf, Proc Natl Acad Sci (PNAS), J Amer Chem Soc (JACS), Biophysical J, Biochimica et Biophysica Acta (General Subjects) Structural Dynamics, J of Artificial Intelligence Research (JAIR), Neural Processing Letters (NEPL), Robotics and Automation Letters (RA-L), IEEE Transactions on Robotics (T-RO), Robotica, IEEE Trans Evol Comput (TEVC), J of Applied Mathematics and Computation, Entropy J, IEEE Trans on Comp Biol and Bioinf (TCBB), IEEE Transactions on NanoBioscience, BMC Structural Biology J, Molecules, J Computer-aided Molecular Design, Proteome Science J, Evolutionary Bioinformatics, Computational Biology and Chemistry J, Intl J Mol Sciences, Computers in Biology and Medicine, Computational and Mathematical Methods in Medicine, J Chem Info and Model, J Comput Chemistry, Molecular Biology Reports, and more.

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[13]Publon Metrics: 96th percentile among reviewers in computer science with 0.1:1 ratio of reviews to publications.

† Conference paper referee for AAAI, NeurIPS, ACM Bioinformatics and Computational Biology Conference (ACM BCB), IEEE Bioinformatics and Biomedicine (BIBM), Intl Conf Res Comp Mol Biol(RECOMB), Intelligent Systems Mol Biol (ISMB), Intl Conf on Bioinf and Comput Biol (BiCoB), Symposium on Computational Geometry (SoCG), Comput Struct Biol Workshop (CSBW), Intl Conf Comp Sys Bioinf (CSB), Intl Workshop Algo Found of Robotics (WAFR), IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS) Inlt Conf Bio-inspired Models of Network, Info, and Comput (Bionetics) IEEE Intl Conf Net Dig Tech (NDT)

Professional Association Membership:

† American Association for Advancement of Science (AAS)
† IEEE, ACM
† American Institute for Medical and Biological Engineering (AIMBE)
† International Society for Computational Biology (ICSB)
† Biophysical Society
† Protein Society
† American Chemical Society (ACS)
† National Council on Undergraduate Research (NCUR)

Other Professional Service and Outreach Activities:

† Steering Committee member, Impact AI Symposium, Northern Virginia Technology Council (NVTC), 2024.

† Panelist, Roundtable Discussion on Standards in the Executive Order in Artificial Intelligence, Center for Strategic and International Studies, January 30, 2024, Washington D.C.

† Panelist, "AI Applications: Biological Systems", Foundations of Machine Learning and its Applications for Scientific Discovery in Physical and Biological Systems Workshop, June 23, 2022, Tysons Corner, VA.

† Panelist, "Responsible AI", NVTC Impact AI, May 11, 2022, Tysons Corner, VA.

† Judge, Student AI Research Proposals, Ideaventions Academy for Mathematics and Science, December 17, 2020, Reston, VA.

† Panelist, "Future of the Architectural Profession as it Related to Data Science, Machine Learning, and AI", AIA Leadership Series, D.C. Local Chapter, 2019, Arlington, VA.

† Panelist, "Ready or Not, Artificial Intelligence and Machine Learning Arrive", Government IT Sales Summit 2018, Reston, VA.

† ISCB Youth Bioinformatics Conference (YBS), panelist, George Mason University, January 12, 2019.

† "Undergraduate research highlights" section contributor of ACM SIGBio newsletter, 2017.

† Judge in Computer Science Category of the (international) Undergraduate Awards, 2017-2015

† Executive Supporter of Girls Computing League, 2016-2015.

† Women in Bioinformatics Panel Member at ACM BCB, 2014.

† George Mason University NSF CAREER panelist, May 20, 2014.

† State Department 3rd Young Scientist Forum, People to People Exchange, September 18, 2012.

† George Mason University NSF CAREER panelist, April 18, 2012.

† Women in Bioinformatics Panel Member at ACM BCB, 2012.

† Organizer of Chantilly High School Bioengineering Tour, June 17, 2011.

† Co-organizer of High School Bioengineering Summer Internship Program, Summer 2011.

† Two-body Problem Panel Member at Grace Hopper Conference, October 2009.

Professional Development Activities:

† Yale School of Management Women's Leadership Program, April 06 – May 18, 2022
† High Threat Security Overseas Training, NSF 2020, 2019
† Bullying in the Workplace Training, Harassment Training, Merit Review Board I-IV Training, NSF 2019
† Conflict of Interest Training, IT Security Training, NSF 2020, 2019
† NIH National Centers For Systems Biology (NCSB) Annual Meeting, July 11-12, 2013
† NSF Grants Conference, October 22-23, 2012
† NSF CISE Career Writing Workshop, Norfolk, VA, April 15, 2011
† NSF Early Career Writing Workshop, Williamsburg, June 2, 2010
† AASCU Proposal Development Workshop, Washington D.C., February 25-27, 2010