

Amarda Shehu

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EMPLOYMENT

George Mason University

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
Faculty co-creator (with Prof. Fei Li), Network Science group	January 2017 – present
Faculty Member, Mason Nanotechnology Initiative	August 2012 – present

EDUCATION

Rice University, Houston, TX

Ph.D. in Computer Science December 2004 to July 2008
Dissertation Title: “*Molecules in Motion: Computing Structural Flexibility*”
Committee: Kavradi LE (dissertation director), Vardi M, Clementi C, and Nakhleh L.

Rice University, Houston, TX

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

Clarkson University, Potsdam, NY

B.S. in Computer Science January 2000 to May 2002
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

RESEARCH FOCUS

The Shehu laboratory focuses on developing novel algorithms to bridge between computer science, engineering, and the life sciences. Our research emphasis is on problem solving, search, optimization, planning, and machine learning to simulate, analyze, and characterize complex dynamic systems operating in the presence of constraints. Our application domains are diverse, spanning from bioinformatics and computational biology and biophysics, to human-computer interaction, and computer-aided engineering design.

SELECTED AWARDS

(in reverse chronological order of date of award)

George Mason University Teaching Excellence Award, 2018.
Outstanding Teaching Award, Department of Computer Science, GMU, 2018.
Distinguished Service Award, Department of Statistics, GMU, 2017.
George Mason University Emerging Researcher/Scholar/Creator Award, 2014.

ACM Service Award in recognition of contributions to ACM-BCB, 2013.
George Mason University OSCAR Mentor Excellence Award, 2013.
Honorable Mention, Humies Competition Award, ACM GECCO, 2012.
Young Faculty Research Award, Department of Computer Science, 2012.

Recipient of 2007-2005 NIH Predoctoral Fellowship, Nanobiology Training Program; 2002-2000 Clarkson University Presidential Scholarship; 2001 Phi-Mu-Epsilon Fellowship Award for “Best Clarkson University student in Computer Science and Mathematics”; 2001 Clarkson University Recognition Day award, Hamlin/Darraugh award, and International Student Excellence Award; 1997 Honorable mention at International Competition of Mathematics, Turkey; 1994-1998 Winner of National Mathematics Olympiad, Albania.

METRICS AT A GLANCE

Scholarly Activity (as of September 06, 2018):

1374 citations, h-index of **22**², i10-index of **45**³

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

²Largest number h s.t. h publications have $\geq h$ citations

³Number of publications with ≥ 10 citations

EXTERNAL FUNDING

(in reverse chronological order of beginning date of award)

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 Supplement 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.
10. REU Supplement 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

(in reverse chronological order of beginning date of award)

- 8 GMU Multidisciplinary Seed Funding Initiative in Modeling, Simulation, and Data Analytics for “An Integrative Multi-disciplinary Approach to Unravel and Target Viral Replication,” \$40K (notified of award on September 07, 2017). 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,” \$10,000, 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,” \$20,000, 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,” \$4,000, 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,” \$12,000, 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,” \$35,000, 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,” \$8,000, 01/01/2009-12/31/2009.
PI: **Shehu A**.

REFEREED PUBLICATIONS

JOURNAL PUBLICATIONS (PEER-REVIEWED)⁴

- 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 Genomics* 2018, in press. [IF: 3.729]
- 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* 2018, in press. [IF: 7.307]
- J41. Akhter N^g and **Shehu A***. *From Extraction of Local Structures of Protein Energy Landscapes to Improved Decoy Selection in Template-free Protein Structure Prediction*. *Molecules* 23(1): 216, 2018. [IF: 2.861]
- J40. Maximova T^p, Zhang Z, Carr DB, Plaku E, and **Shehu A***. *Sample-based Models of Protein Energy Landscapes and Slow Structural Rearrangements*. *J Comput Biol* 25(1):33-50, 2017. [IF: 1.03]
- J39. Sapin E^p, De Jong K*, and **Shehu A***. *From Optimization to Mapping: An Evolutionary Algorithm for Protein Energy Landscapes*. *IEEE/ACM Trans Comput Biol and Bioinf* 15(3):719-731, 2018. [IF: 1.96]
- J38. Maximova T^p, Plaku E*, and **Shehu A***. *Structure-guided Protein Transition Modeling with a Probabilistic Roadmap Algorithm*. *IEEE/ACM Trans Comput Bio and Bioinf*, 2017.
(doi: 10.1109/TCBB.2016.2586044) [IF: 1.96]
- J37. Veltri D^g, Kamath U, and **Shehu A***. *Improving Recognition of Antimicrobial Peptides and Target Selectivity through Machine Learning and Genetic Programming*. *IEEE/ACM Trans Comput Biol and Bioinf* 14(2):1545-5963, 2017. [IF: 1.54]
- J36. **Shehu A*** and Plaku E*. *A Survey of Computational Treatments of Biomolecules by Robotics-inspired Methods Modeling Equilibrium Structure and Dynamics*. *J Artif Intel Res* 597: 509-572, 2016. [IF: 0.91]
- J35. Sapin E^p, Carr DB, De Jong K*, and **Shehu A***. *Computing energy landscape maps and structural excursions of proteins*. *BMC Genomics* 17(Suppl 4): 546, 2016. [IF: 3.99]
- J34. Molloy K^g, Clausen R^g, and **Shehu A***. *A Stochastic Roadmap Method to Model Protein Structural Transitions*. *Robotica* 34(8): 1705-1733 (featured on [issue cover](#)), 2016. [IF: 0.89]
- J33. Molloy K^g and **Shehu A***. *A General, Adaptive, Roadmap-based Algorithm for Protein Motion Computation*. *IEEE Trans NanoBioScience* 15(2): 158-165, 2016. [IF: 1.77]

⁴Articles 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.

- J32. Maximova T^p, Moffat R^g, Ma B, Nussinov R, and **Shehu A***. *Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics*. *PLoS Comput Biol* 12(4): e1004619, 2016, (top 50 most downloaded for 2016 and featured on issue cover and PLoS Comput Biol blog). [IF: 4.83]
- J31. **Shehu A*** and Nussinov R*. *Computational Methods for Exploration and Analysis of Macromolecular Structure and Dynamics*. *PLoS Comput Biol* 11(10): e1004585, 2015 (editorial). [IF: 4.83]
- J30. Devaurs D, Molloy K^g, Vaisset M, **Shehu A**, Simeon T, and Cortes J*. *Characterizing Energy Landscapes of Peptides using a Combination of Stochastic Algorithms*. *IEEE Trans NanoBioScience* 14(5): 545-552, 2015. [IF: 1.77]
- J29. Hashmi I^g and **Shehu A***. *idDock+: Integrating Machine Learning in Probabilistic Search for Protein-protein Docking*. *J Comput Biol* 22(9): 806-822, 2015. [IF: 1.67]
- J28. Clausen R^g and **Shehu A***. *A Data-driven Evolutionary Algorithm for Mapping Multi-basin Protein Energy Landscape*. *J Comput Biol* 22(9): 844-860, 2015. [IF: 1.67]
- J27. Clausen R^g, Ma B, Nussinov R*, and **Shehu A***. *Mapping the Conformation Space of Wildtype and Mutant Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm*. *PLoS Comput Biol* 11(9): e1004470, 2015. [IF: 4.83]
- J26. Kamath U^g, De Jong KA*, and **Shehu A***. *Effective Automated Feature Construction and Selection for Classification of Biological Sequences*. *PLoS One* 9(7): e99982, 2014. [IF: 5.2]
- J25. Molloy K^g, Van JM^u, Barbara D, and **Shehu A***. *Exploring Representations of Protein Structure for Automated Remote Homology Detection and Mapping of Protein Structure Space*. *BMC Bioinf*, 15(Suppl 8): S4, 2014. [IF: 3.02]
- J24. Kabbani, N*, Nordman JC, Corgiat B, Veltri D^g, **Shehu A**, and Adams DJ. *Are Nicotinic Receptors Coupled to G Proteins?* *Bioessays*, 35(12):1025-1034, 2013 ([video abstract](#)). [IF: 5.42]
- J23. Ashoor A, Nordman JC, Veltri D^g, Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Lupica C, **Shehu A**, Kabbani N, and Oz M*. *Menthol Inhibits 5-HT₃ Receptor-mediated Currents*. *J of Pharmacology and Experimental Therapeutics* 347(20):398-409, 2013 ([issue front cover](#)). [IF: 4.31]
- J22. Ashoor A, Nordman JC, Veltri D^g, Yang KS, Al Kury L, Shuba Y, Mahgoub M, Howarth FC, Sadek B, **Shehu A**, Kabbani N, and Oz M*. *Menthol Binding and Inhibition of Alpha7-nicotinic Acetylcholine Receptors*. *PLoS One* (8)7:e67674, 2013 (top 25% most cited as of June 2017). [IF: 4.09]
- J21. Molloy M^g, Saleh S^u, and **Shehu A***. *Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab-initio Protein Structure Prediction*. *IEEE/ACM Trans Comput Biol and Bioinf*, 10(5):1162-1175, 2013. [IF: 2.25]
- J20. Hashmi I^g and **Shehu A***. *HopDock: A Probabilistic Search Algorithm for Decoy Sampling in Protein-protein Docking*. *Proteome Sci* 11(Suppl 1):S6, 2013. [IF: 2.42]
- J19. Saleh S^u, Olson B^g, and **Shehu A***. *A population-based Evolutionary Search Approach to the Multiple Minima Problem in de novo Protein Structure Prediction*. *BMC Struct Biol* 13(Suppl 1): S4, 2013. [IF: 2.10]
- J18. Olson B^g and **Shehu A***. *Rapid Sampling of Local Minima in Protein Energy Surface and Effective Reduction through a Multi-objective Filter*. *Proteome Sci* 11(Suppl 1):S12, 2013. [IF: 2.42]
- J17. Molloy M^g and **Shehu, A***. *Elucidating the Ensemble of Functionally-relevant Transitions in Protein Systems with a Robotics-inspired Method*. *BMC Struct Biol* 13(Suppl 1):S8, 2013. [IF: 2.09]
- J16. Olson B^g, Hashmi I^g, Molloy K^g and **Shehu, A***. *Basin Hopping as a General and Versatile Optimization Framework for the Characterization of Biological Macromolecules*. *Advances in Artificial Intelligence J*, 674832, 2012 (special issue1 on applications in biomedicine).
- J15. Olson B^g and **Shehu A***. *Evolutionary-inspired Probabilistic Search for Enhancing Sampling of Local Minima in the Protein Energy Surface*. *Proteome Sci*, 10(Suppl1): S5, 2012. [IF: 2.42]
- J14. Hashmi I^g, Akbal B, Haspel N, and **Shehu A***. *Guiding Protein Docking with Geometric and Evolutionary Information*. *J Bioinf and Comp Biol*, 10(3): 1242008, 2012. [IF: 1.06]
- J13. Akbal B, Hashmi I^g, **Shehu A**, and Haspel N*. *An Evolutionary Conservation Based Method for Refining and Reranking Protein Complex Structures*. *J Bioinf and Comp Biol*, 10(3): 12420024, 2012. [IF: 1.06]
- J12. Olson B^g, Molloy^g, K, Hendi S-F^g, and **Shehu A***. *Guiding Probabilistic Search of the Protein Conformational Space with Structural Profiles*. *J Bioinf and Comp Biol*, 10(3): 1242005, 2012. [IF: 1.06]

- J11. **Shehu A*** and Kavraki LE*. *Modeling Structures and Motions of Loops in Protein Molecules*. *Entropy J*, 14(2):252-290, 2012 (invited review article). [IF: 1.11]
- J10. Kamath U^g, Compton J^u, Islamaj-Dogan R, De Jong KA*, and **Shehu A***. *An Evolutionary Algorithm Approach for Feature Generation from Sequence Data and its Application to DNA Splice-Site Prediction*. *IEEE Trans Comput Biol and Bioinf*, 9(5):1387-1398, 2012. [IF: 2.25]
- J9. Kamath U^g, **Shehu A***, and De Jong KA*. *A Two-Stage Evolutionary Approach for Effective Classification of Hypersensitive DNA Sequences*. *J Bioinf and Comp Biol*, 9(3):399-413, 2011. [IF: 1.06]
- J8. Olson B^g, Molloy K^g and **Shehu A***. *In Search of the Protein Native State with a Probabilistic Sampling Approach*. *J Bioinf and Comp Biol*, 9(3):383-398, 2011. [IF: 1.06]
- J7. **Shehu A*** and Olson B^g. *Guiding the Search for Native-like Protein Conformations with an Ab-initio Tree-based Exploration*. *Intl J of Robot Res*, 29(8):1106-1127, 2010. [IF: 4.93]
- J6. Hegler JA, Laetzer J, **Shehu A**, Clementi C, and Wolynes, PG*. *Restriction vs. Guidance: Fragment Assembly and Associative Memory Hamiltonians for Protein Structure Prediction*. *Proc Natl Acad Sci USA*, 106(36):15302-15307, 2009. [IF: 9.54]
- J5. **Shehu A**, Clementi C*, and Kavraki LE*. *Multiscale Characterization of Protein Conformational Ensembles*. *Proteins: Struct Funct Bioinf*, 76(4):837-851, 2009. [IF: 3.03]
- J4. **Shehu A**, Kavraki LE, and Clementi C*. *Unfolding the Fold of Cyclic Cysteine-rich Peptides*. *Protein Sci* 17(3):482-493, 2008. [IF: 3.11]
- J3. **Shehu A**, Clementi C, and Kavraki LE*. *Sampling Conformation Space to Model Equilibrium Fluctuations in Proteins*. *Algorithmica* 48(4):303-327, 2007. [IF: 0.89]
- J2. **Shehu A**, Kavraki LE, and Clementi C*. *On the Characterization of Protein Native State Ensembles*. *Biophys J* 92(5):1503-1511, 2007. [IF: 4.53]
- J1. **Shehu A**, Clementi C*, and Kavraki LE*. *Modeling Protein Conformational Ensembles: From Missing Loops to Equilibrium Fluctuations*. *Proteins: Struct Funct Bioinf* 65(1):164-179, 2006. [IF: 3.88]

CONFERENCE PUBLICATIONS (PEER-REVIEWED)

- C36. Nasrin Akhter^g, Gopinath Chennupati, Hristo Djidjev, and **Shehu A***. *Improved Decoy Selection via Machine Learning and Ranking*. IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), Las Vegas, Nevada 2018 (accepted).
- C35. Akhter N^g and **Shehu A***. *Analysis of Energy Landscapes for Improved Decoy Selection in Template-free Protein Structure Prediction*. In Proc Intl Conf on Bioinf and Comp Biol (BiCoB), Las Vegas, NV 2018, *nominated for best paper*.
- C34. Morris D^g, Maximova T^p, Plaku E, and **Shehu A***. *Out of One, Many: Exploiting Intrinsic Motions to Explore Protein Structure Spaces*. In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), Orlando, FL 2017, accepted.
- C33. Qiao W, Maximova T^p, Fang, X^u, and **Shehu A***. *Reconstructing and Mining Protein Energy Landscape to Understand Disease*. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Kansas City, MO 2017, pg. 22-27. [AR: 19%]
- C32. Sapin E^p, De Jong KA, and **Shehu A***. *Modeling Protein Structural Transitions as a Multi-objective Optimization Problem*. In Proc IEEE Intl Conf on Comput Intel in Bioinf and Comput Biol (CIBCB), Manchester, England, 2017, pg.1-8, isbn: 978-1-4673-8988-4.
- C31. Maximova T^p, Carr DB, Plaku E, and **Shehu A***. *Sample-based Models of Protein Structural Transitions*. In Proc ACM Conf on Bioinf and Comp Biol (BCB), Seattle, WA, 2016, pg. 128-137. [AR: 20%]
- C30. Sapin E^p, De Jong KA, and **Shehu A***. *A Novel EA-based Memetic Approach for Efficiently Mapping Complex Fitness Landscapes*. In Proc Genet and Evol Comp Conf (GECCO), Denver, CO, 2016, pg. 85-92. [AR: 40%]
- C29. Pandit R^h and **Shehu A***. *A Principled Comparative Analysis of Dimensionality Reduction Techniques on Protein Structure Decoy Data*. In Proc Intl Conf on Bioinf and Comp Biol (BiCoB), Las Vegas, NV, 2016, pg. 43-48. [AR: 40%]
- C28. Maximova T^p, Plaku E*, and **Shehu A***. *Computing Transition Paths in Multiple-Basin Proteins with a Probabilistic Roadmap Algorithm Guided by Structure Data*. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Washington, D.C., 2015, pg. 35-42. [AR: 19%]

- C27. Sapin E^p, De Jong KA, and **Shehu A***. *Evolutionary Search Strategies for Efficient Sample-based Representations of Multiple-basin Protein Energy Landscapes*. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Washington, D.C., 2015, pg. 13-20. [AR: 19%]
- C26. Molloy K^g and **Shehu A***. *Interleaving Global and Local Search for Protein Motion Computation*. In Lecture Notes in Computer Science: Bioinformatics Research and Applications, vol. 9096, pg. 175-186 (Proc 11th Intl Symp Bioinf Res & Appl – ISBRA) Norfolk, VA, 2015, vol 9096, pg. 175-186. [AR: 30%]
- C25. Clausen R^g, Sapin E^p, De Jong KA, and **Shehu A***. *Evolution Strategies for Exploring Protein Energy Landscapes*. In Proc Genet and Evol Comp Conf (GECCO), Madrid, Spain, 2014, pg. 217-224. [AR: 50%]
- C24. Veltri D^g, Kamath U, and **Shehu A***. *A Novel Method to Improve Recognition of Antimicrobial Peptides through Distal Sequence-based Features*. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014, pg. 371-378 (*Best Student Paper Award*). [AR: 19%]
- C23. Devaurs D, **Shehu A***, Simeon T and Cortes S. *Sampling-based Methods for a Full Characterization of Energy Landscapes of Small Peptides*. In Proc IEEE Intl Conf on Bioinf and Biomed (BIBM), Belfast, UK, 2014, pg. 37-44. [AR: 19%]
- C22. Clausen R^g and **Shehu A***. *A Multiscale Hybrid Evolutionary Algorithm to Obtain Sample-based Representations of Multi-basin Protein Energy Landscapes*. In Proc ACM Conf on Bioinf and Comp Biol (BCB), Newport Beach, CA, 2014, pg. 269-278. [AR: 25%]
- C21. Hashmi I^g, Veltri D^g, Kabbani N, and **Shehu A***. *Knowledge-based Search and Multiobjective Filters: Proposed Structural Models of GPCR Dimerization*. In Proc ACM Conf on Bioinf and Comp Biol (BCB), Newport Beach, CA, 2014, pg. 279-288. [AR: 25%]
- C20. Olson, B^g and **Shehu A***. *Multi-Objective Optimization Techniques for Conformational Sampling in Template-Free Protein Structure Prediction*. In Proc Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014, pg. 1-6. [AR: 40%]
- C19. Molloy, K^g and **Shehu A***. *A Probabilistic Roadmap-based Method to Model Conformational Switching of a Protein Among Many Functionally-relevant Structures*. In Proc Intl Conf on Bioinf and Comp Biol (BICoB), Las Vegas, NV, 2014, pg. 1-6 (*finalist for Best Paper Award*). [AR: 40%]
- C18. Randou E, Veltri D^g, and **Shehu A***. *Binary Response Models for Recognition of Antimicrobial Peptides*. In Proc ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C. 2013, pg. 76-85. [AR: 20%]
- C17. Olson B^g, and **Shehu A***. *Multi-Objective Stochastic Search for Sampling Local Minima in the Protein Energy Surface*. In Proc ACM Conf on Bioinf and Comp Biol (BCB), Washington, D. C. 2013, pg. 430-439. [AR: 20%]
- C16. Randou E, Veltri D^g, and **Shehu A***. *Systematic Analysis of Global Features and Model Building for Recognition of Antimicrobial Peptides*. In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013, pg. 1-6. [AR: 42%]
- C15. Molloy K^g, Van JM^u, Barbara D, and **Shehu A***. *Higher-order Representations for Automated Organization of Protein Structure Space*. In Proc IEEE Intl Conf on Comput Adv in Bio and Medical Sciences (ICCABS), New Orleans, LA, 2013, pg. 287-294. [AR: 42%]
- C14. Olson B^g, De Jong KA, and **Shehu A***. *Off-Lattice Protein Structure Prediction with Homologous Crossover*. In Proc Genet and Evol Comp Conf (GECCO), Amsterdam, Netherlands, 2013. [AR: 36%]
- C13. Veltri D^g and **Shehu A***. *Physicochemical Determinants of Antimicrobial Activity*. In Proc Intl Conf on Bioinf and Comput Biol, (BICoB), Hawaii, 2013, pg. 1-6. [AR: 20%]
- C12. Hashmi I^g and **Shehu A***. *A Basin Hopping Algorithm for Protein-Protein Docking*. In Proc IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM) 2012, Philadelphia, PA, pg. 466-469. [AR: 20%]
- C11. Molloy K^g and **Shehu A***. *Biased Decoy Sampling to Aid the Selection of Near-Native Protein Conformations*. In Proc ACM Bioinf and Comp Biol (BCB), Orlando, FL, 2012, pg. 131-138. [AR: 21%]
- C10. Olson B^g and **Shehu A***. *Efficient Basin Hopping in the Protein Energy Surface*. In Proc IEEE Conference on Bioinformatics and Biomedicine (BIBM), Philadelphia, PA, 2012, pg. 119-124. [AR: 20%]
- C9. Kamath U^g, Kaers J, **Shehu A** and De Jong KA*. *A Spatial EA Framework for Parallelizing Machine Learning Methods*. In Proc Intl Conf on Parallel Problem Solving From Nature (PPSN), Taormina, Italy, 2012, LNCS vol. 7491, pg. 206-215. [AR: 47%]

- C8. Olson B^g and **Shehu A***. *Populating Local Minima in the Protein Conformational Space*. In Proc IEEE Intl Conference on Bioinformatics and Biomedicine (BIBM), Atlanta, GA, 2011, pg. 114-117. [AR: 20%]
- C7. Kamath U^g, De Jong KA*, and **Shehu A***. *An Evolutionary-based Approach for Feature Generation: Eukaryotic Promoter Recognition*. In Proc IEEE Congress on Evolutionary Computation (CEC), New Orleans, LA, 2011, pg. 277-284. [AR: 51%]
- C6. Olson B^g, Molloy K^g, and **Shehu A***. *Enhancing Sampling of the Conformational Space Near the Protein Native State*. In Proc Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 249-263, (*Best Student Paper Award*). [AR: 24%]
- C5. Kamath U^g, **Shehu A***, and De Jong KA*. *Feature and Kernel Evolution for Recognition of Hypersensitive Sites in DNA Sequences*. In Proc Intl. Conference on Bio-inspired Models of Network, Information, and Computing Systems (BIONETICS), Boston, MA, 2010, LNICST (Springer), vol. 87, pg. 213-238. [AR: 24%]
- C4. Kamath U^g, **Shehu A***, and De Jong KA*. *Using Evolutionary Computation to Improve SVM Classification*. In Proc IEEE World Congress on Computational Intelligence (WCCI), Barcelona, Spain, 2010, pg. 1-8. [AR: 67%]
- 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)

- 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)

- 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 ABSTRACTS⁵

- A68. Roychoudhury 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*)

⁵Abstracts 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.

- 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). *Outstanding Research Presentation Award*.
- 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, Massachusetts, 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, Frederick, 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 PUBLICATIONS⁶

- 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.

⁶These are not peer-reviewed. In addition to select technical reports, this list includes profiles published in a section I introduced in 2013 to the ACM SIGBIO newsletter. The objective is to feature prominent computer scientists and computational biology researchers and raise awareness in the ACM SIGBIO community.

INVITED TALKS

- 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 Algorithms⁷, 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.

⁷The 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.

- 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.
- 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](#). Additional community dissemination and outreach materials (including research and education) are also available on our webpage.

Selected Source-code, Executables, and Web Servers:

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 Structure 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

TEACHING

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 gauge 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:

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	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:

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. Veltri defended his Ph.D. on December 01, 2015 with 4 journal and 5 conference papers. He is 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. Hashmi defended her Ph.D. on July 27, 2015 with 5 journal, 2 conference, and 3 workshop papers. She is now a term instructor at IST-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. Molloy defended his Ph.D. on January 13, 2015 with 9 journal, 4 conference, and 2 workshop papers. After a postdoctoral fellowship at LAAS-CNRS, Toulouse, he is now an adjunct and software engineer at George Mason 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. Kamath defended his Ph.D. on December 11, 2013 with 6 journal papers, and 7 conference papers, all with Shehu and De Jong as corresponding authors with the exception of 1 conference paper. He is now Chief Data Scientist at BAE Systems Applied Intelligence.
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. Olson defended his Ph.D. on July 24, 2013 with 7 journal, 7 conference, and 3 workshop papers. He is now research scientist at LinkedIn.

M.S. Theses:

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

(as Committee Member)

Gideon Gogovi, CMASC (director: Estela Blaisten-Barojas)	2018-present
Jing Lei, Statistics (director: Wanli Qiao)	2018-present
Joseph Graus, Computer Science (director: Yotam Gingold)	2018-present
Achyuthan J.R., Civil, Environmental, and Infrastructure Engineering (director: David Lattanzi)	2018-2016
Christopher Siwy, School of Systems Biology (director: Dmitri Klimov)	2017-2014
Gregory Helmick, CSI (director: Estela Blaisten-Barojas)	2017-2014
Evan Behar, Computer Science, (director: Jyh-Ming Lien)	2017-2013
Zhonghua Xi, Computer Science (director: Jyh-Ming Lien)	2017-2015

Amarda Shehu	CV-16/22
	2017-2015
	2015-2014
	2013-2012
	2015-2012
	2011

Yoseph Abere, CSI (director: Estela Blaisten-Barojas)
 Jose Colbes, Computer Science CICESE-Mexico, (director: Carlos Brizuela)
 Yanyan Lu, Computer Science, (director: Jyh-Ming Lien)
 Adam Cadien, SPACS, (director: Howard Sheng)
 Nada Basit, Computer Science, (director: Harry Wechsler)

STUDENT ADVISING AND MENTORING

(in research-related activities)

Postdoctoral Fellows:

2. Tatiana Maximova (May 2018 - April 2015)
1. Emmanuel Sapin (December 2016 - January 2015)

Ph.D. Students:⁸

14. Yiyang Lian (Spring 2019 - Fall 2018, Lab rotation)
13. Parastoo Kamranfar (Summer 2018–current)
12. Manpriya Dua (Summer 2018–current)
11. Kazi Lutful Kabir (Summer 2018–current)
10. Zahra Rajabi (Summer 2018–current, co-advising with Hemant Purohit/IST-GMU)
9. Sivani Depal (Summer 2018–current)
8. Ahmed Bin Zaman (Summer 2018–current)
7. Nasrin Akhter (Fall 2017–current)
6. Erich O’Saben (Spring 2016–Spring 2018)
- 5.-1. Ph.D. alumni Daniel Veltri, Irina Hashmi, Kevin Molloy, Uday Kamath, and Brian Olson

M.S. Students:

- | | |
|---|-----------|
| 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:⁹

- | | |
|---|---------------------------|
| 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 |
| 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 |

⁸These students have earned numerous awards during their research in my lab, some of which are highlighted below.

⁹Mentoring 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.

- | | |
|--|---------------------------|
| 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:¹⁰

- | | |
|--|---------------------------|
| 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 from 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):

- | | |
|--|---|
| 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 |
| 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)
<i>Best student paper at IEEE BIBM in first-author capacity</i>
Travel Award, ICCABS
Outstanding Oral Presentation, School of Systems Biology Student Research Day, Daniel Veltri | November 2014
June 2013
May 2013 |
| 15. Irina Hashmi (CS Ph.D., graduated 2015)
Best Poster Award, IEEE BIBM
Travel Awards, IEEE BIBM, CRA-W Grad Cohort Workshop
Research Assistant Fellowship | October 2012
May 2011
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 |

¹⁰I am a Thomas Jefferson Summer/Fall Program Mentor since 2014.

13. Jennifer M. Van (CS undergrad, 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 undergrad, 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:**

Steering/Advisory Board member for the Office of Research Computing at George Mason University, June 2017-present.

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

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), February 17, 2017.

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 NSF CAREER Workshop (panel member), April 28, 2012.

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

Volgenau School of Engineering Service:

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:

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

Member of GMU CS Advisory Council, 2018-2019.

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

Recruitment committee, Spring 2018, Spring 2017.

Mentor of junior faculty, 2017.

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

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

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-present

Graduate Studies Committee, 2016-present

Ph.D. Committee, 2014-present

PAR Evaluation Committee, 2017-present

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-present.

Ph.D. Admissions Committee, George Mason University, 2012-present.

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:

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 Kavradi, 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

Workshop Organization:

15. “Computational Structural Biology Workshop” at ACM BCB, August 20, 2017, Boston, MA.
14. “Women@GECCO” at GECCO, July 15, 2017, Berlin, Germany.
13. “Evolutionary Computation in Computational Biology” at GECCO, July 16, 2017, Berlin, Germany.
12. “Women@GECCO” at GECCO, July 2016, Denver, Colorado.
11. “Evolutionary Computation in Computational Biology” at GECCO, July 2016, Denver, Colorado.
10. “Computational Structural Biology Workshop” at IEEE BIBM, November 11, 2015, Washington, D.C.
9. “Evolutionary Computation in Computational Biology” at GECCO, July 11, 2015, Madrid, Spain.
8. “Computational Structural Biology Workshop” at ACM BCB, September 20, 2014, Newport Beach, LA.
7. “Robotics Methods for Biological Structures and Kinematics Modeling” Workshop at RSS, July 16, 2014 Berkeley, CA.
6. “NSF CISE CAREER Writing Workshop” March 31, 2013, Arlington, VA.
5. “Artificial Intelligence and Robotics Methods in Computational Biology” Workshop at AAAI, July 14, 2013 Bellevue, WA.
4. “Computational Structural Biology Workshop” at ACM BCB, September 22, 2013, Washington, D.C.
3. “Computational Structural Biology Workshop” at IEEE BIBM, October 4, 2012, Philadelphia, PA.
2. “Computational Structural Biology Workshop” at IEEE BIBM, November 12, 2011, Atlanta, GA.
1. “Evolutionary Computation and Machine Learning in Bioinformatics Workshop” (BioLearn) at BIONETICS, Dec. 1-3, 2010, Boston, MA.

Tutorial Organization

7. “Modeling Macromolecular Structures and Motions: Computational Methods for Sampling and Analysis of Energy Landscapes” at ACM BCB 2018, Washington, DC.
6. “Robotics-inspired Algorithms for Modeling Protein Structures and Motions” at ACM BCB 2017, Boston, MA.
5. “Evolutionary Algorithms for Protein Structure Modeling” at ACM BCB, October 2016, Seattle, Washington.
4. “Evolutionary Algorithms for Protein Structure Modeling” at GECCO, July 11, 2015, Madrid, Spain.
3. “Robot Motion Planning Methods for Modeling Structures and Motions of Biomolecules” at ACM BCB, September 20, 2014, Newport Beach, CA.
2. “Evolutionary Search Algorithms for Protein Modeling: From De-novo Structure Prediction to Comprehensive Maps of Functionally-relevant Structures of Protein Chains and Assemblies” at GECCO, July 12, 2014, Vancouver, Canada.
1. “From Robot Motion Planning to Modeling Structures and Motions of Biological Molecules” at ACM BCB, September 22, 2013, Washington, D.C.

Other Chairships:

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

Editorial Positions:

- 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).

Grant Proposal Referee:

NSF, 2018, 2017, 2016, 2015, 2013, 2012, 2011

NIH, 2018, 2017, 2016, 2015

Accelerating Scientific Discovery (ASDI) (Netherlands e-Science Center + Netherlands Organisation for Scientific Research), 2016

AgreenSkills (EU + INRIA), 2014-2013

Journal Referee (in past five years):

2017: PLoS Comput Biol, Molecules, Comput Biol and Chem

2016: Structure, PLoS Comput Biol, Proteins: Struct Funct Bioinf, BMC Bioinf, Mol Biol Reports, Structural Dynamics, Comput Biol and Chem, Computers in Biol and Med, F1000Research, IEEE Trans Evol Comput, J Appl Soft Comput, J Bioinf and Comput Biol.

2015: FEBS Letters, Biophysica et Biochimica Acta, Scientific Reports, PLoS Comput Biol, Proteins: Struct Funct and Bioinf, Comput Biol and Chem J, IEEE Trans NanoBioScience, J of Artificial Intelligence Research (JAIR), IEEE Transactions on Evol Comput (TVEC), Int J Mol Sci.

2014: BMC Genomics, Journal of the Royal Society Interface, Computers in Biology and Medicine, J of Artificial Intelligence Research (JAIR), Proteins: Struct Funct and Bioinf, IEEE/ACM Trans on Comp Biol and Bioinf (TCBB).

2013: J of Artificial Intelligence Research (JAIR), IEEE Transactions on Robotics (T-RO), J of Applied Mathematics and Computation, IEEE/ACM Trans on Comp Biol and Bioinf (TCBB), BMC Structural Biology J, Proteome Sci.

2012: PLoS Comp Biol, Entropy J, Computational and Mathematical Methods in Medicine, J Chem Info and Model, Comput and Struct Biotechnology J, J Bioinf and Comp Biol (JBCB).

Conference Referee (in past five years):

2017: IEEE BIBM, IEEE ICCABS, Comput Struct Biol Workshop (CSBW).

2016: ISMB, RECOMB, ACM BCB, IEEE BIBM, IEEE ICCABS.

2015: RECOMB, IEEE BIBM.

2014: ACM BCB, Comput Struct Biol Workshop (CSBW), BICoB.

2013: Symposium on Computational Geometry (SoCG).

2012: ACM BCB, Comput Struct Biol Workshop (CSBW).

Professional Association Membership:

National Council on Undergraduate Research (NCUR)

American Association for Advancement of Science (AAAS)

IEEE, IEEE Robotics and Automation Society, and IEEE Women in Engineering

IEEE CIS BBTC

ACM, SIGBIO, SIGACT, SIGART, SIGSIM, SIGEVO, SIGKDD

International Society for Computational Biology (ICSB)

Biophysical Society

Protein Society

American Chemical Society (ACS)

Mason Nanotechnology Initiative

Other Professional Service and Outreach Activities:

“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:

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